

```
graph LR
    subgraph 5 [ ]
        10[Simulation Module]
        60[Output Module]
        70[Report Module]
        80[(Database)]
        10 <--> 60
        10 <--> 80
        10 --> 70
    end
    70 --> 20[ ]
```

Fig. 1A

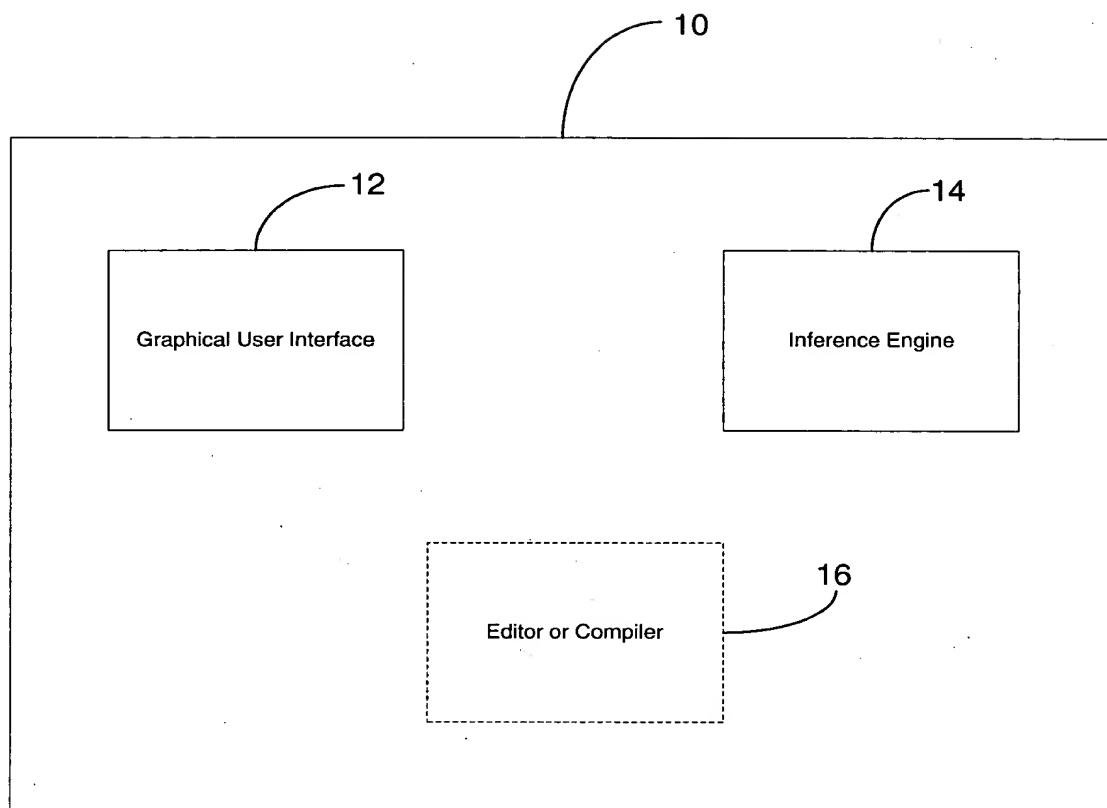
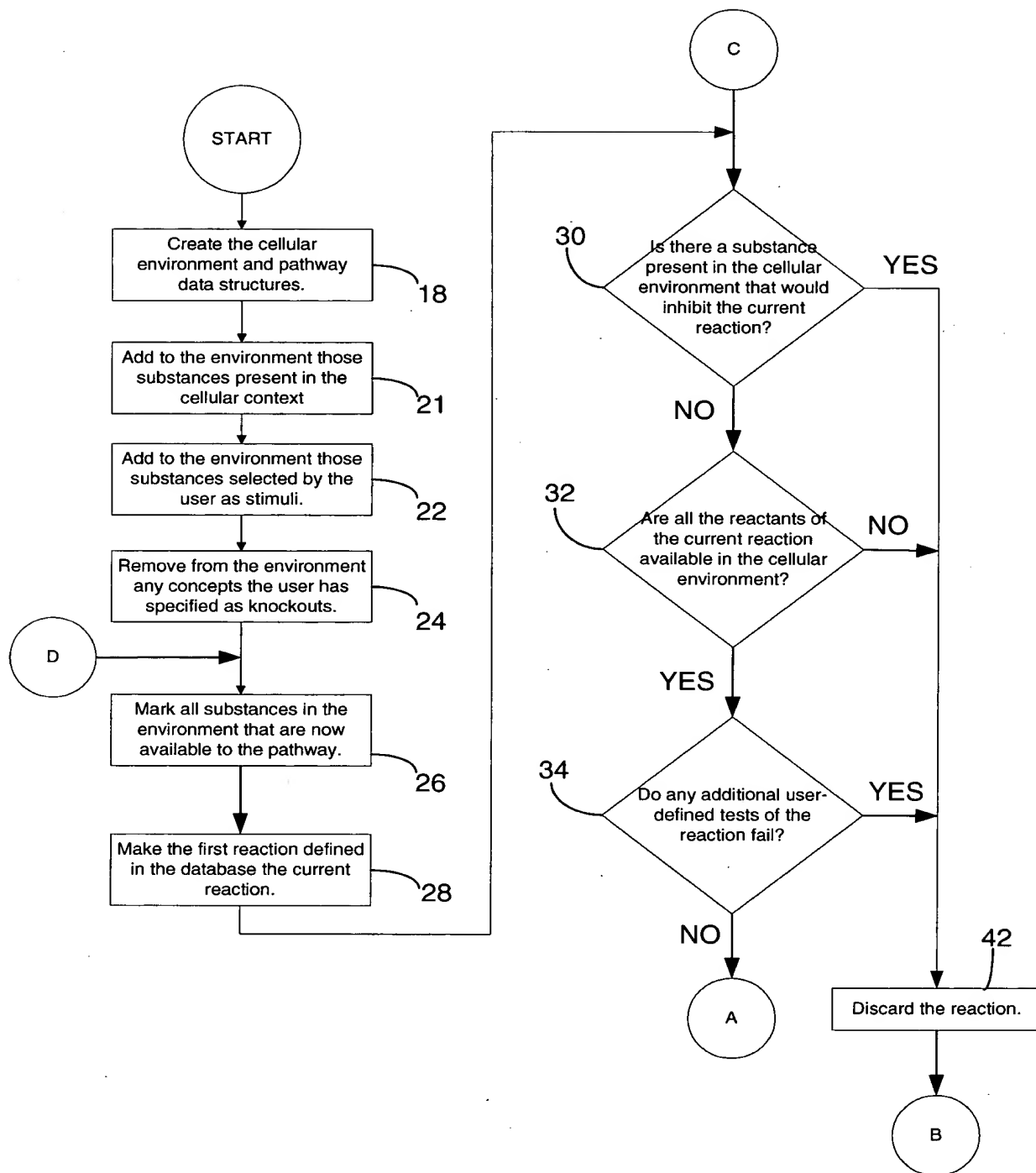


Fig. 1B

Fig. 2A



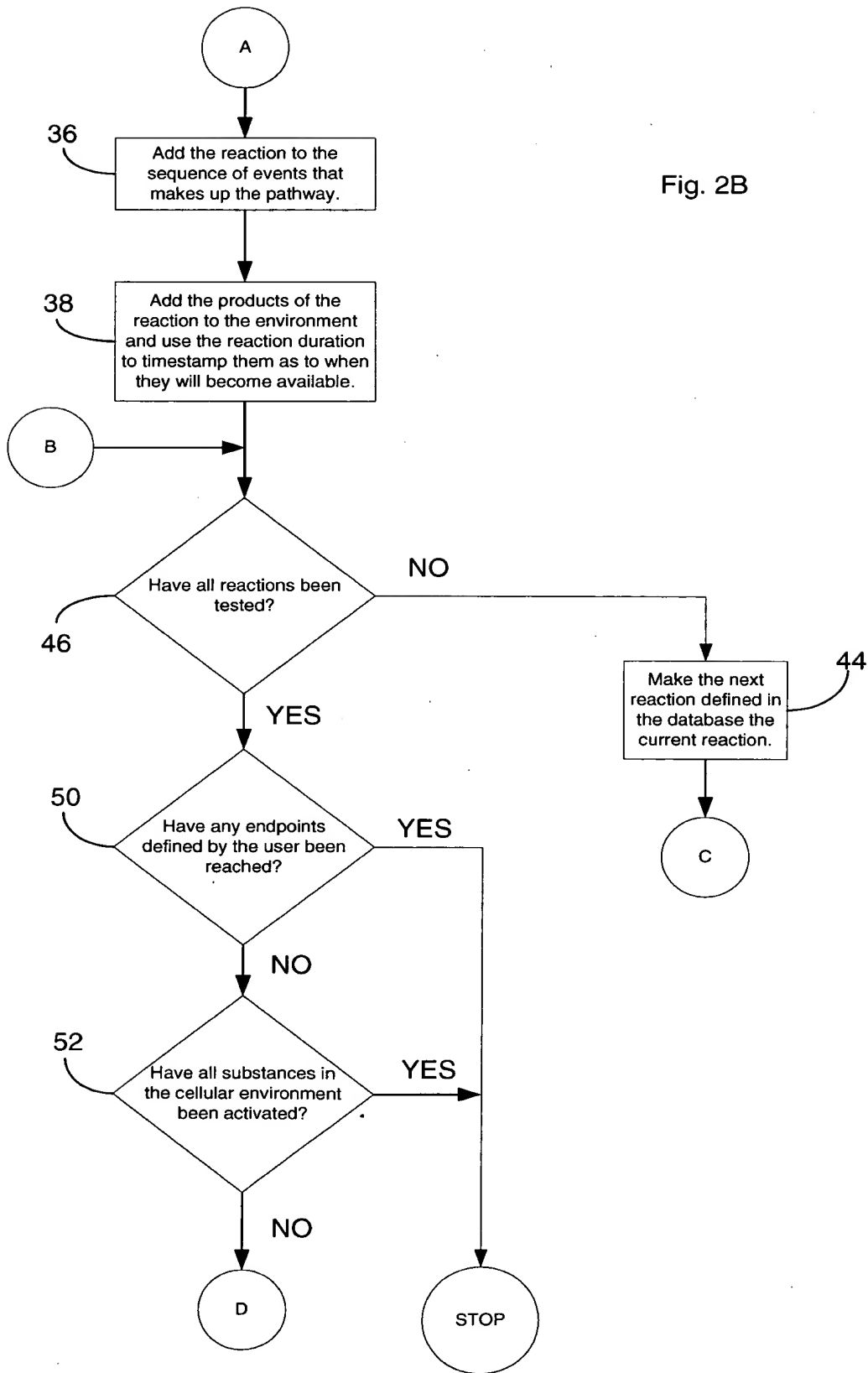


Fig. 2B

Fig. 2C

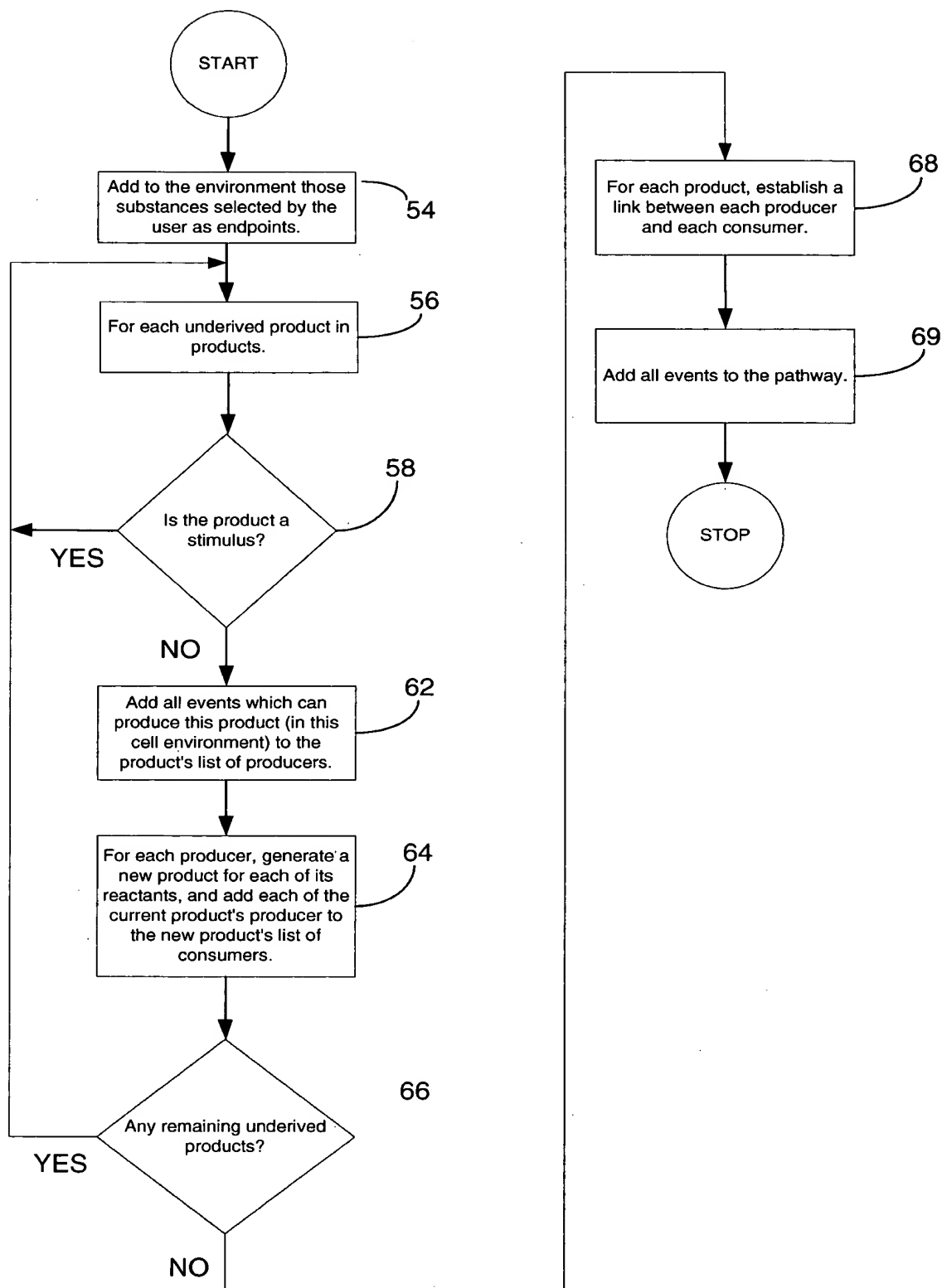


FIGURE 3

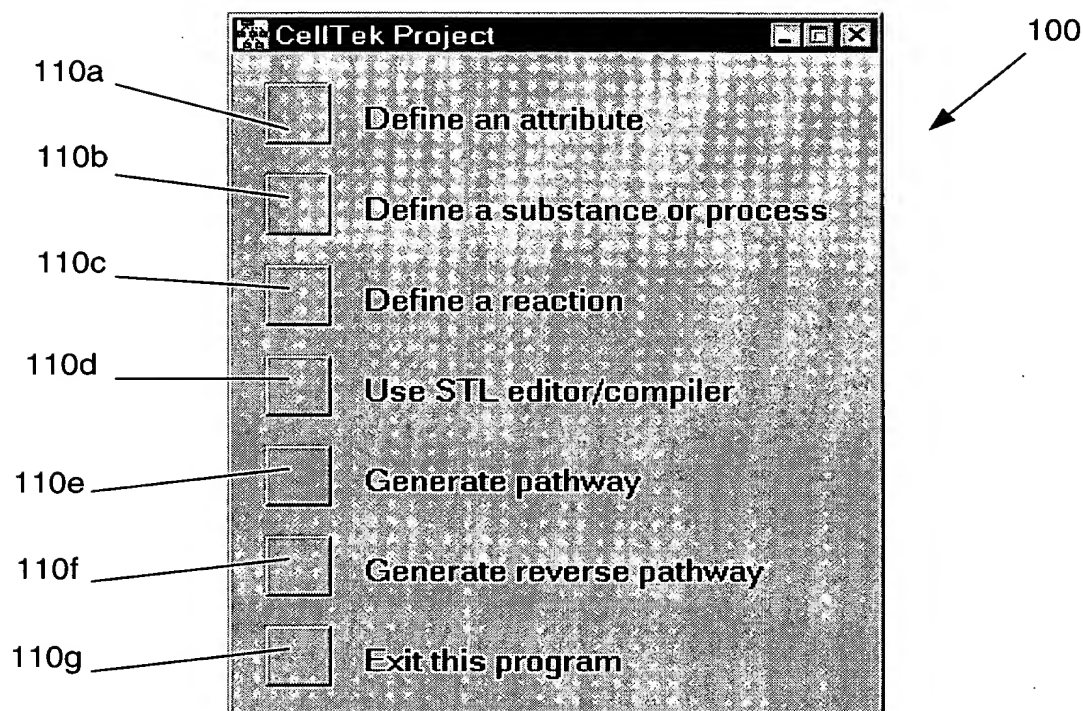


FIGURE 4A

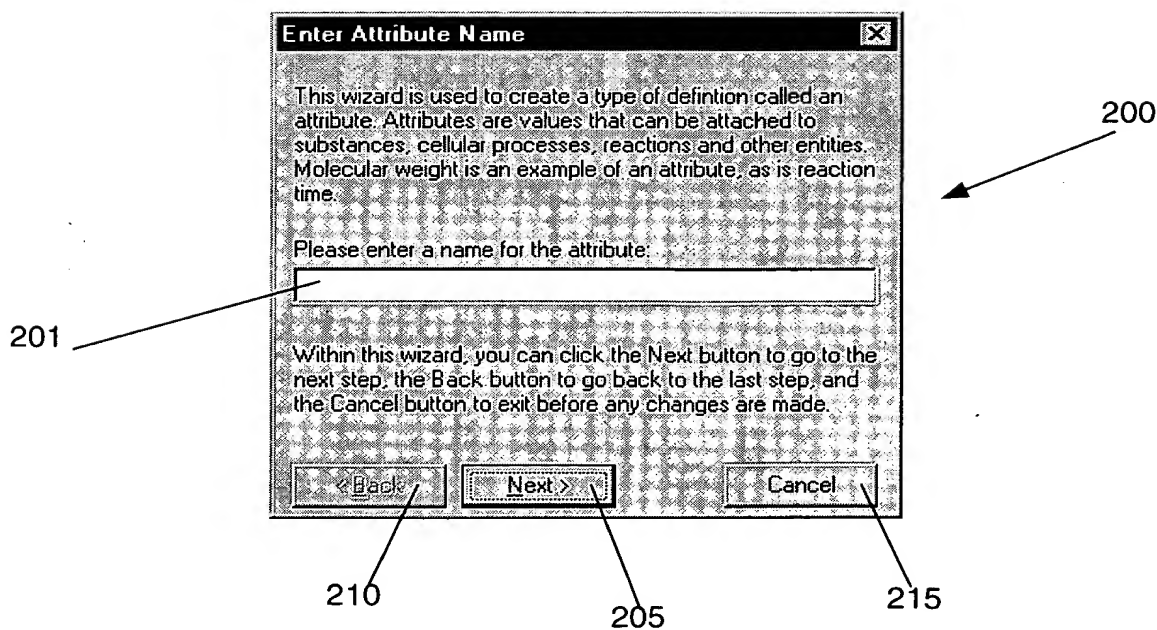


FIGURE 4B

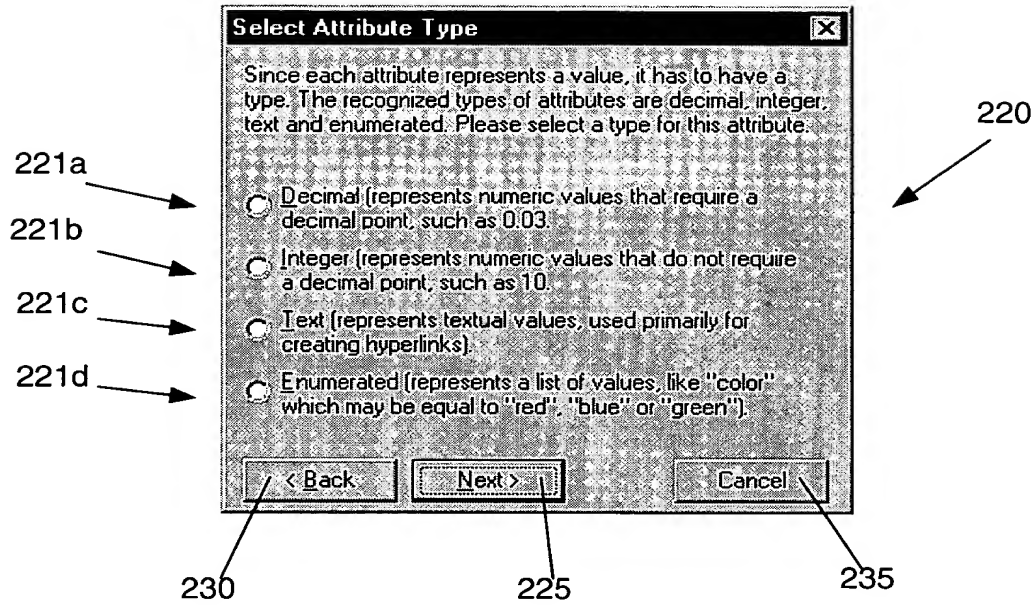


FIGURE 4C

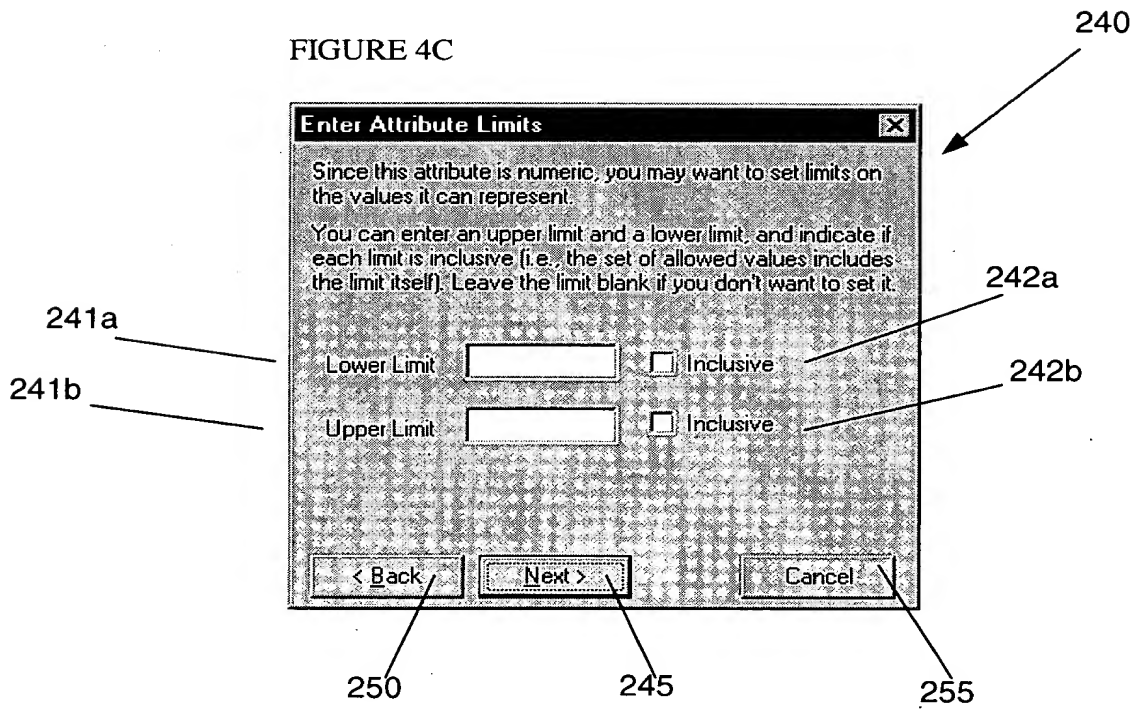


FIGURE 4D

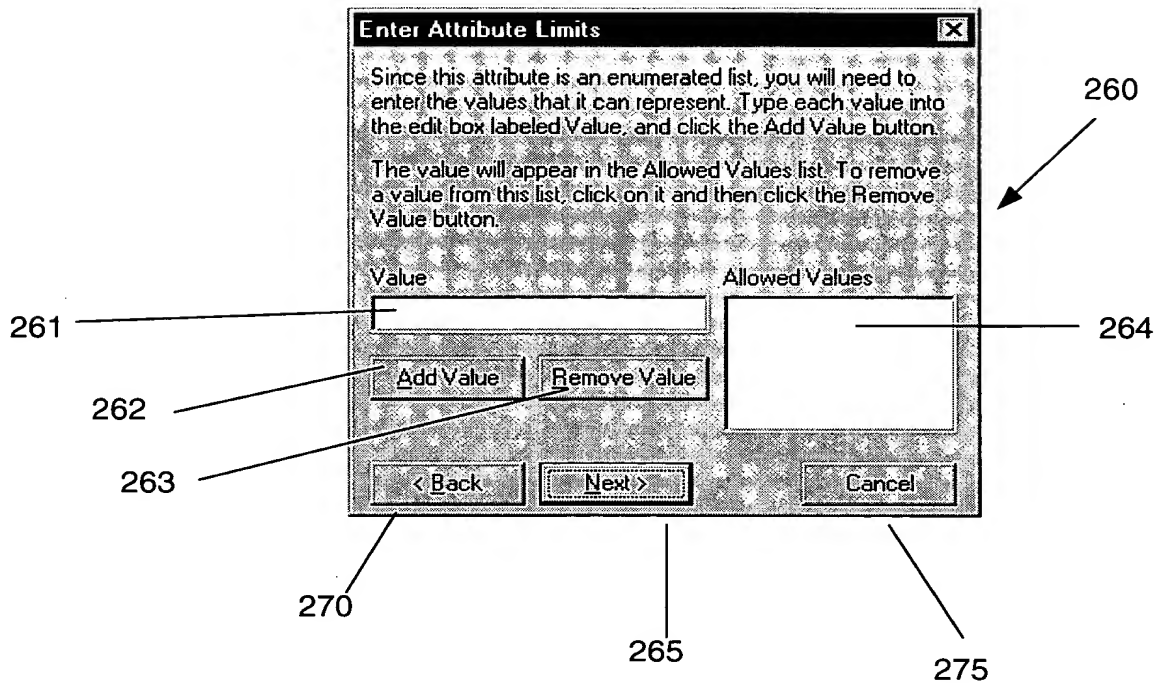


FIGURE 4E

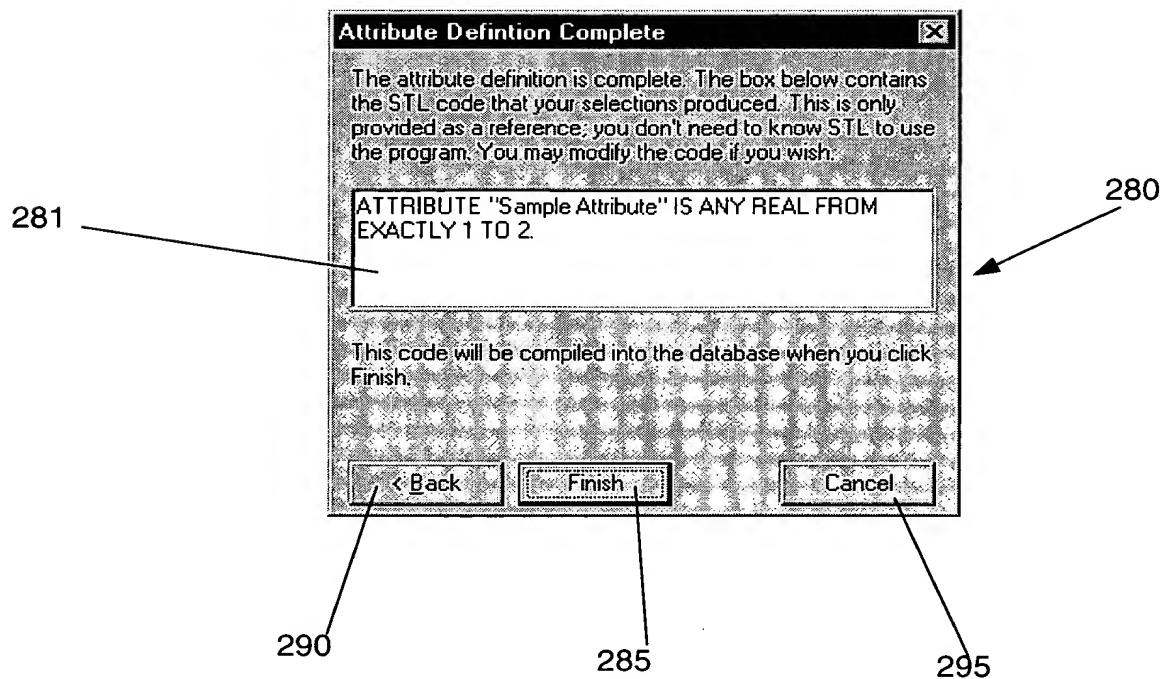


FIGURE 5A

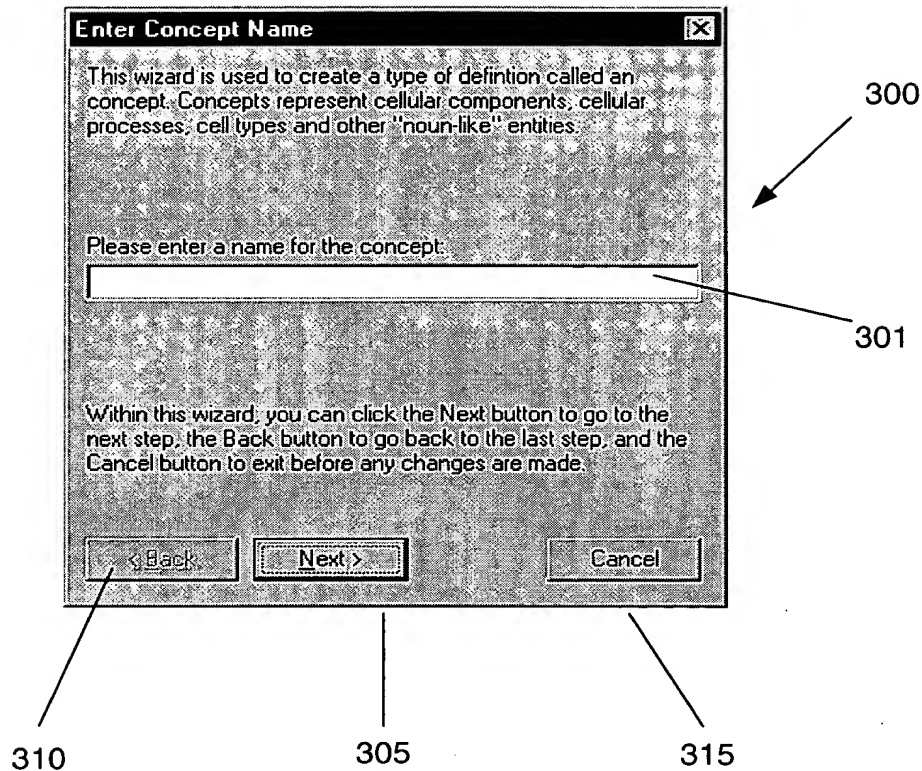


FIGURE 5B

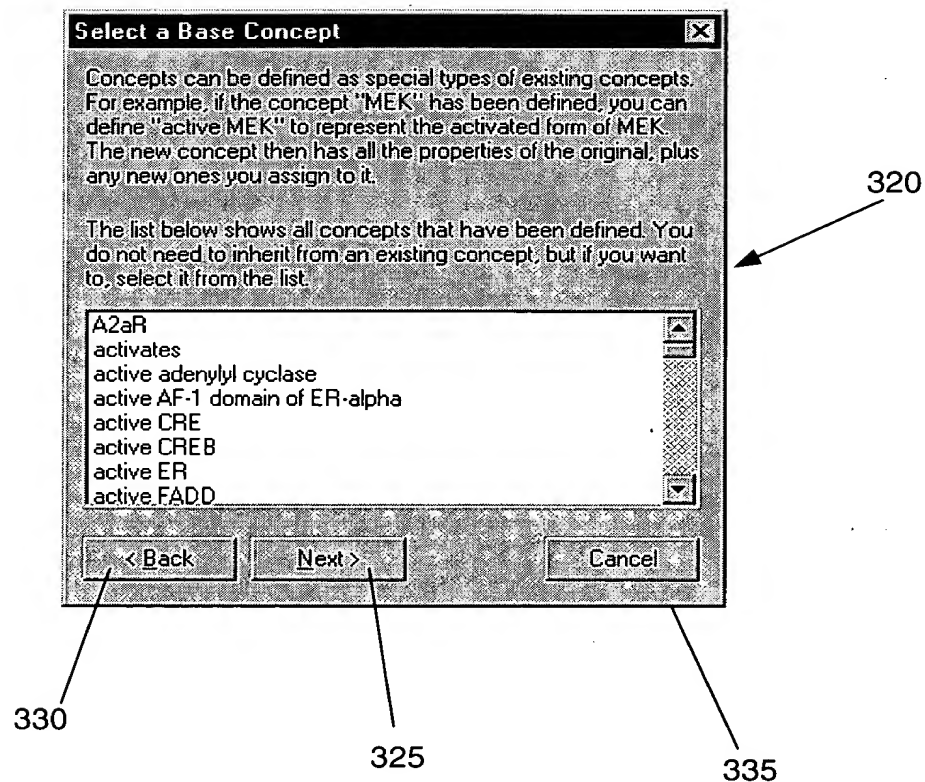


FIGURE 5C

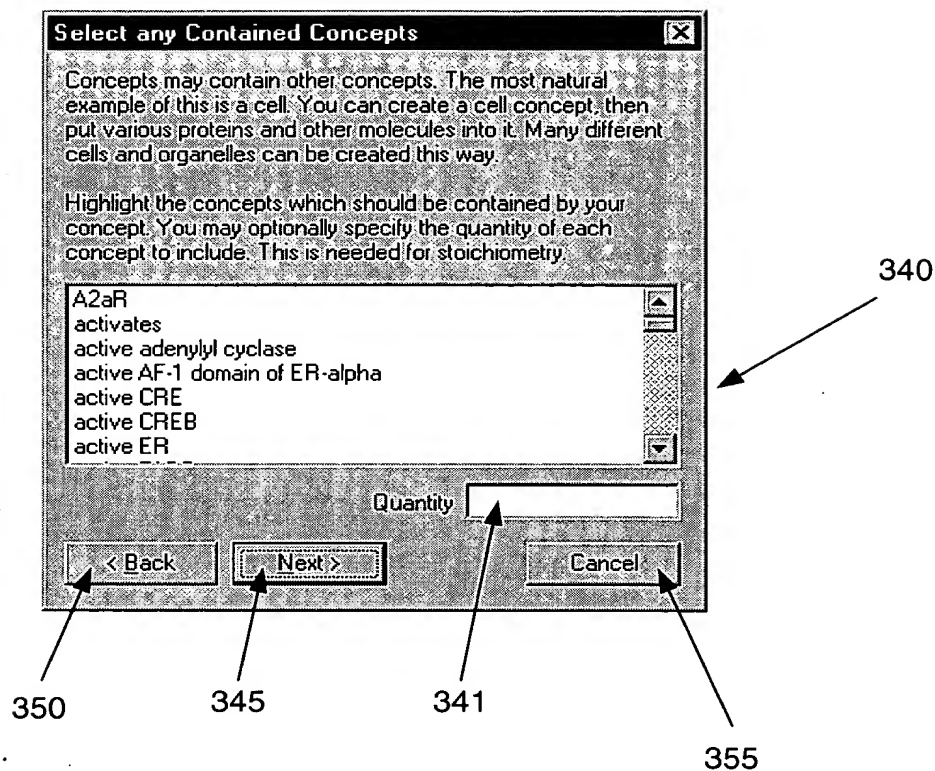


FIGURE 5D

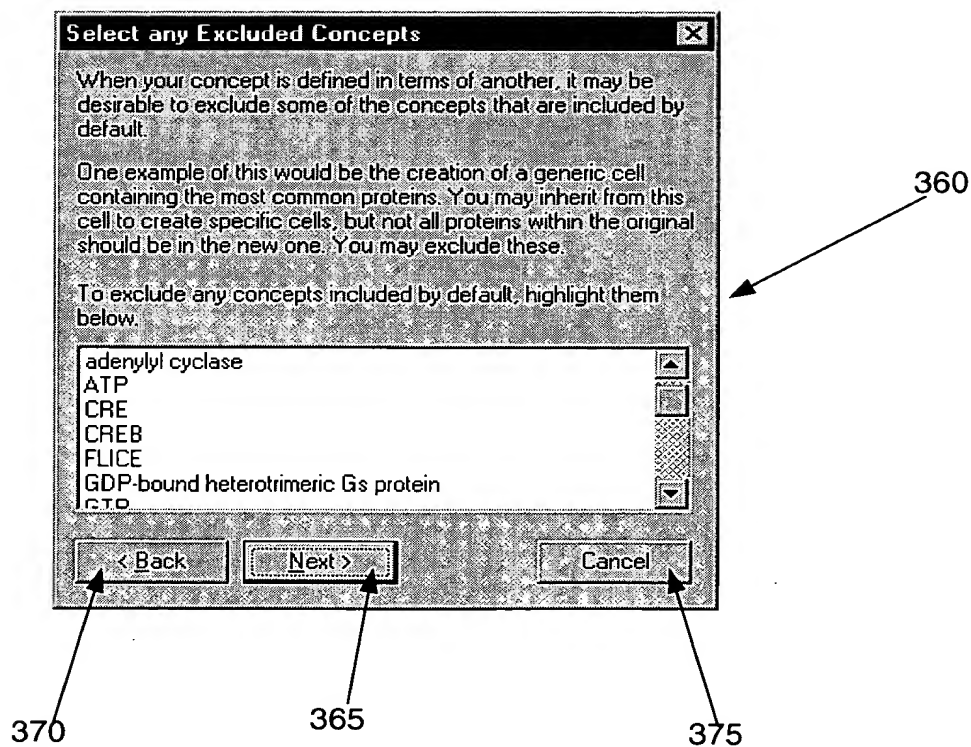


FIGURE 5E

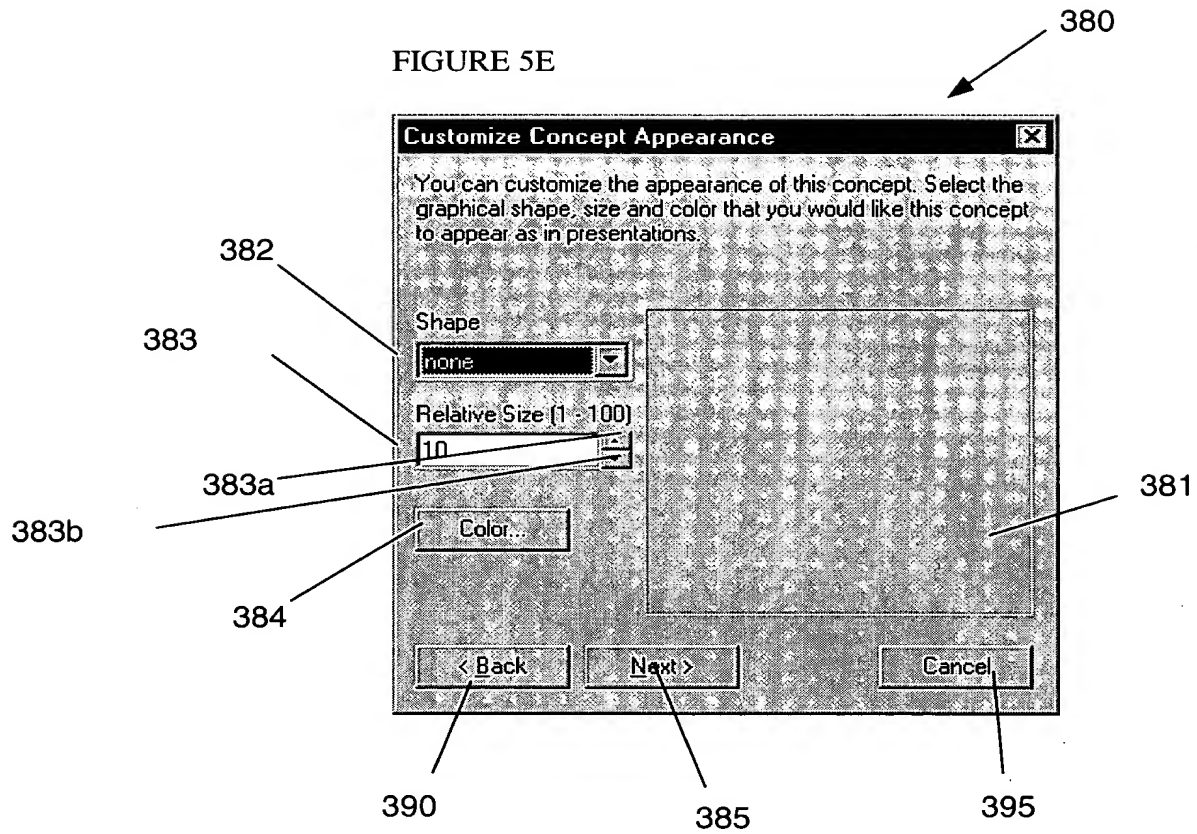


FIGURE 5F

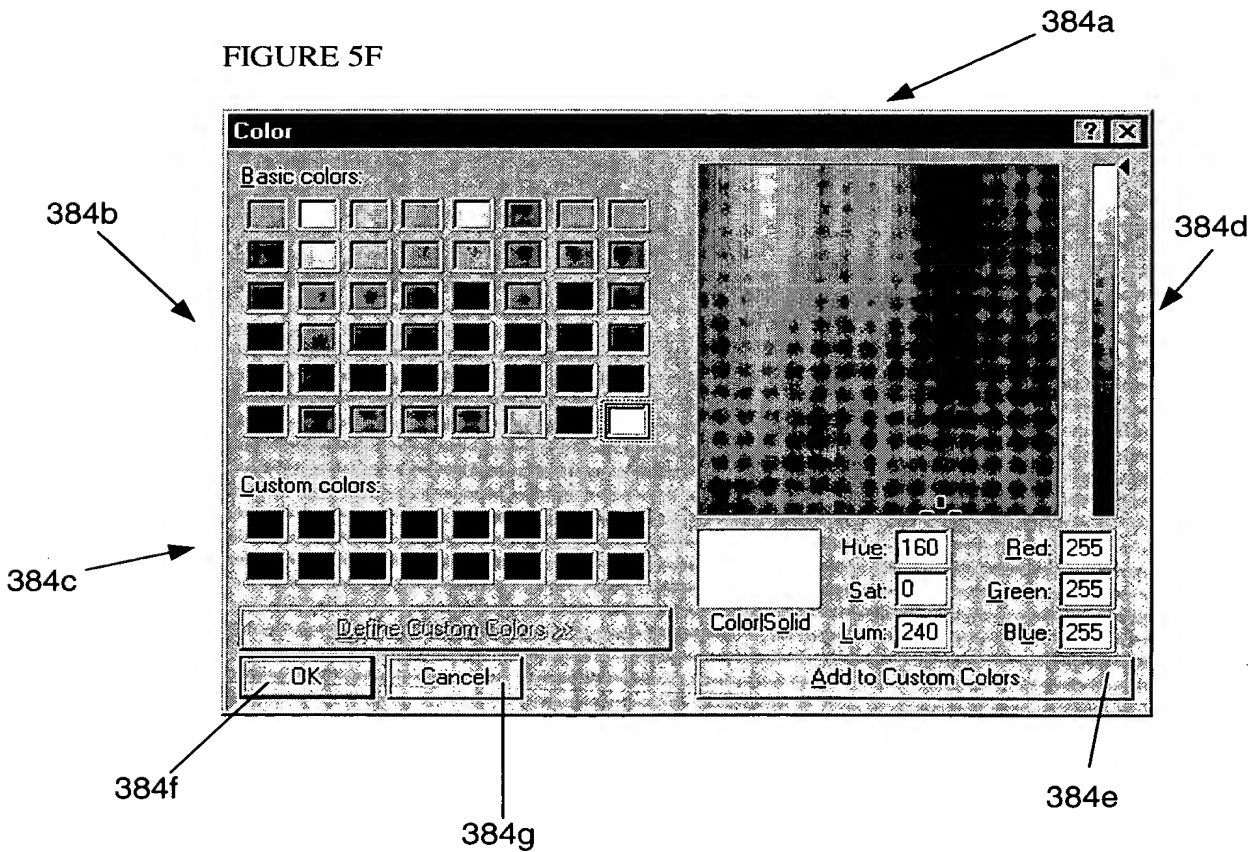


FIGURE 5G

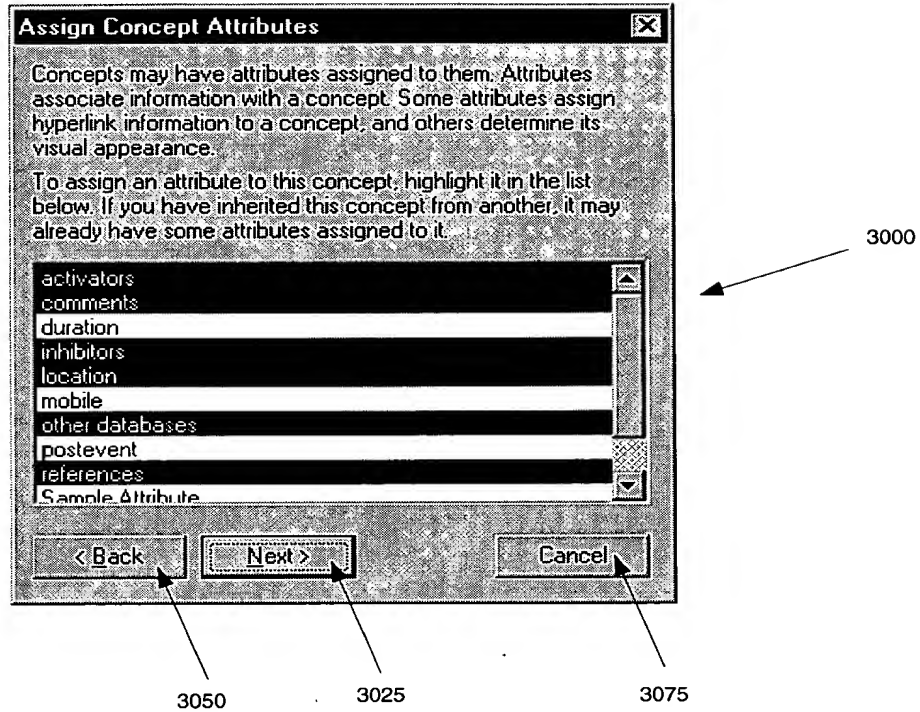


FIGURE 5H

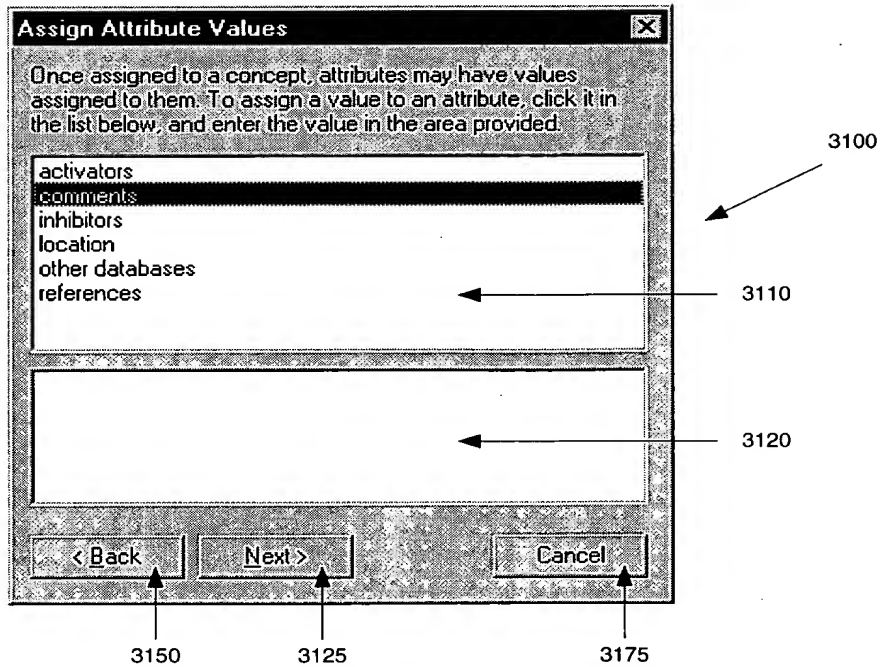


FIGURE 5I

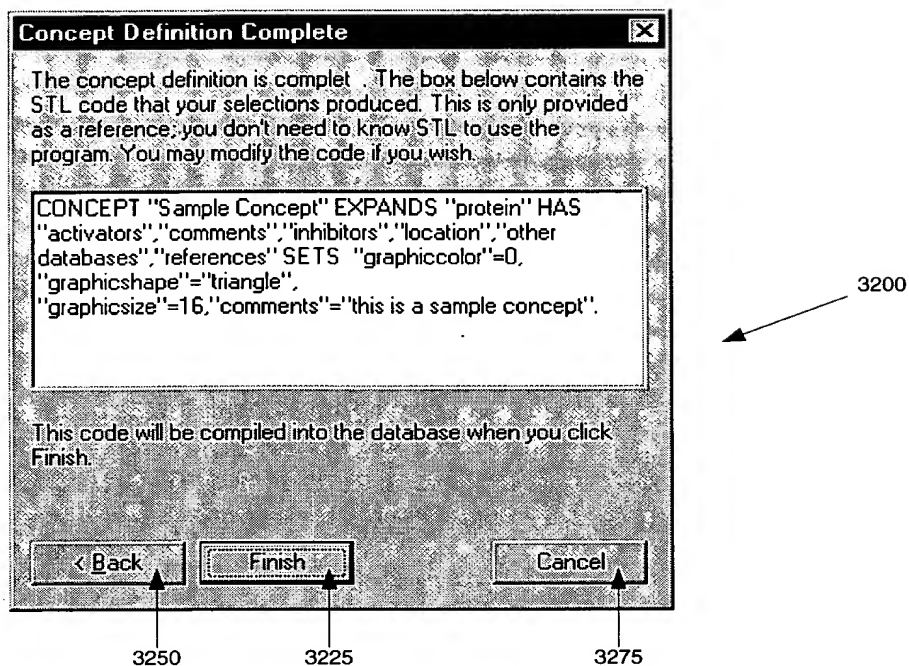


FIGURE 6A

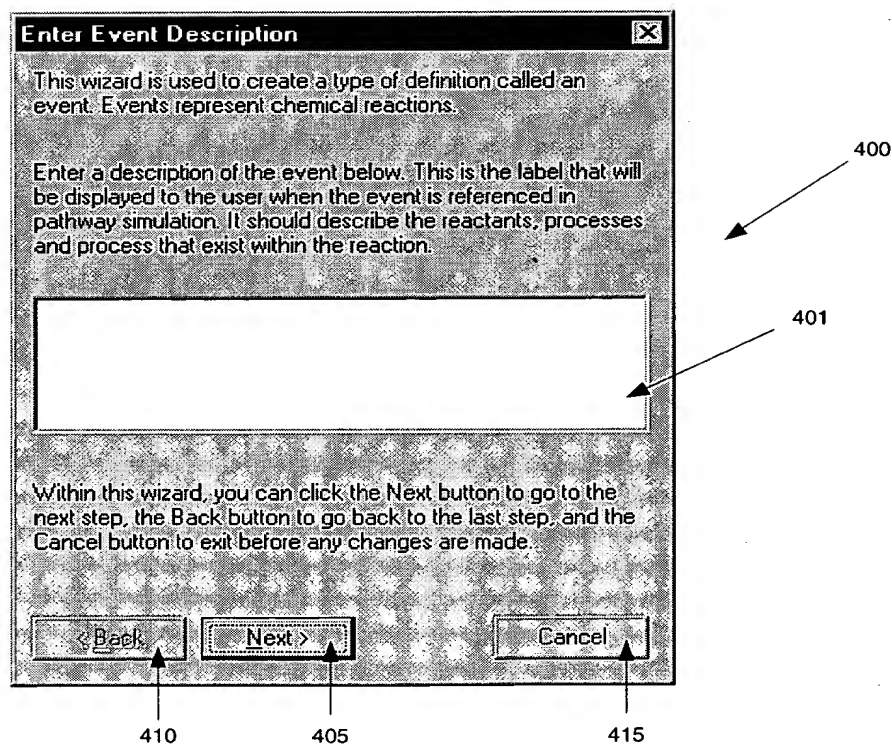


FIGURE 6B

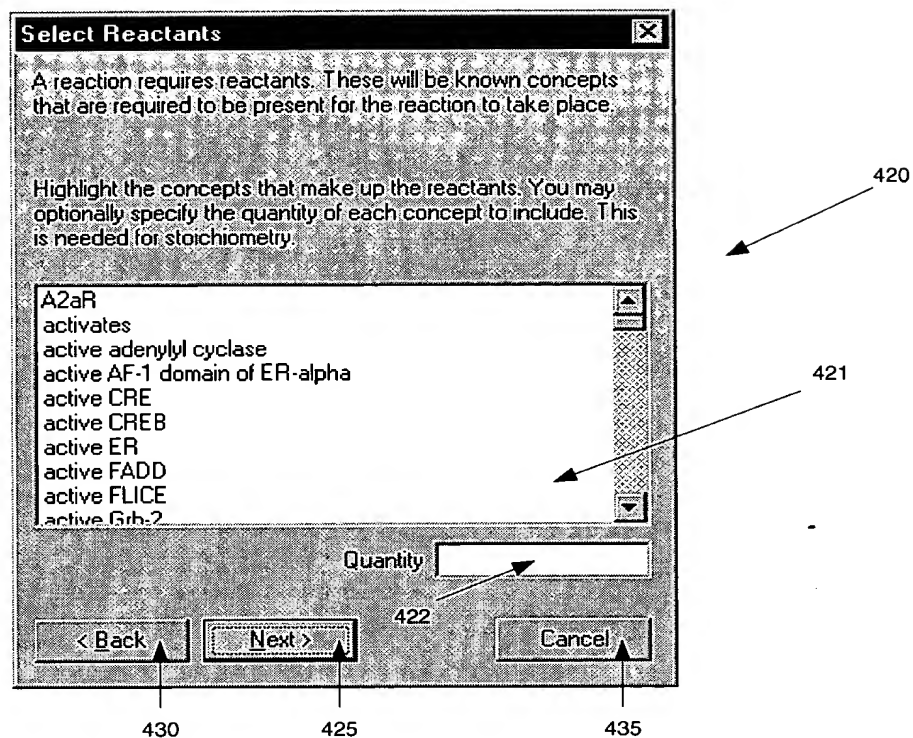


FIGURE 6C

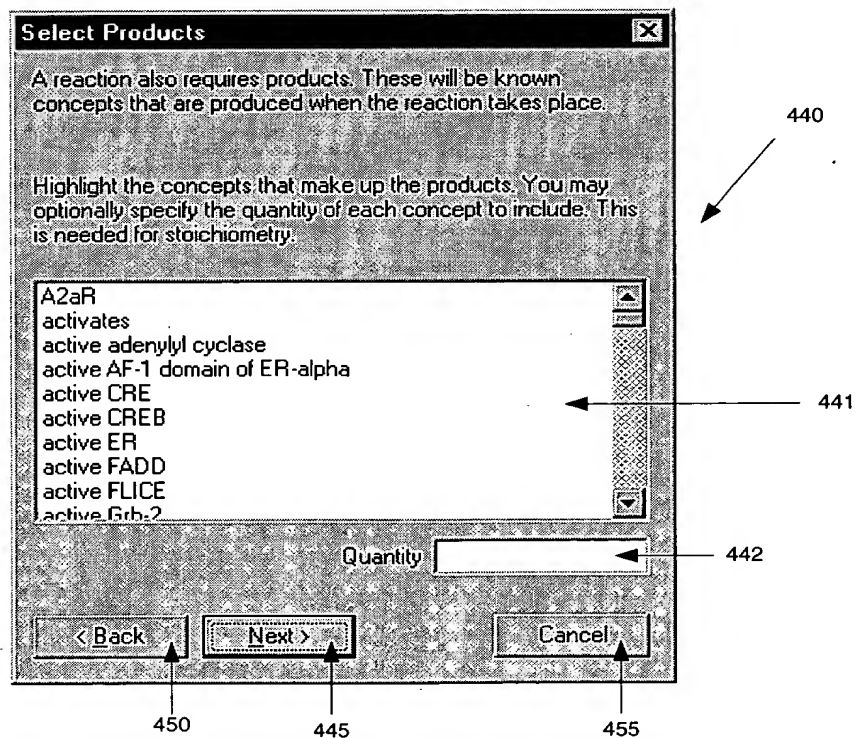


FIGURE 6D

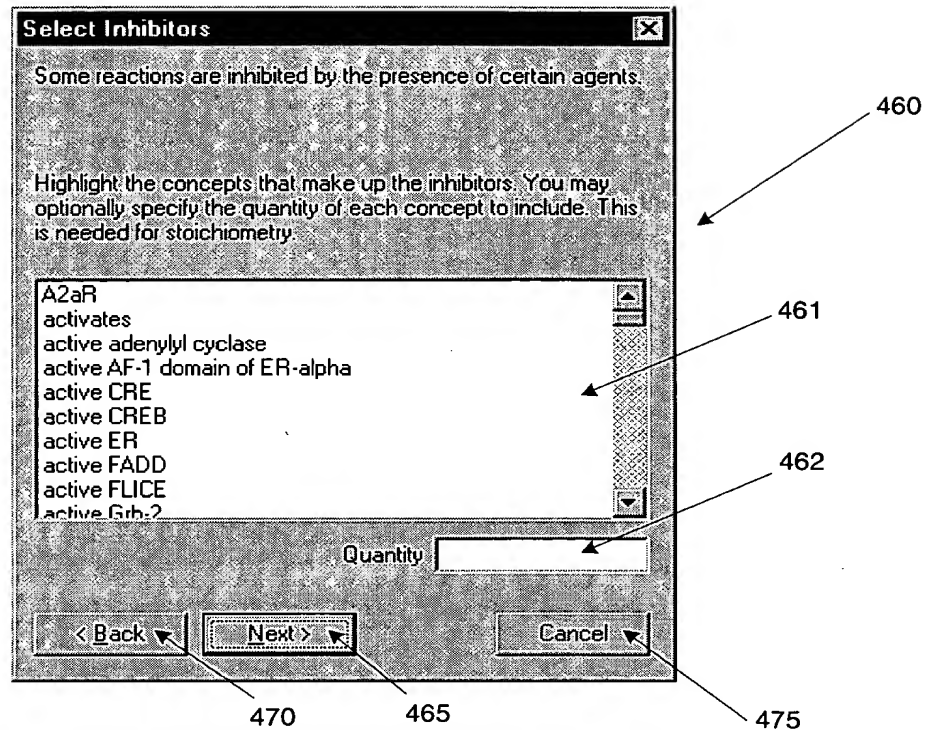


FIGURE 6E

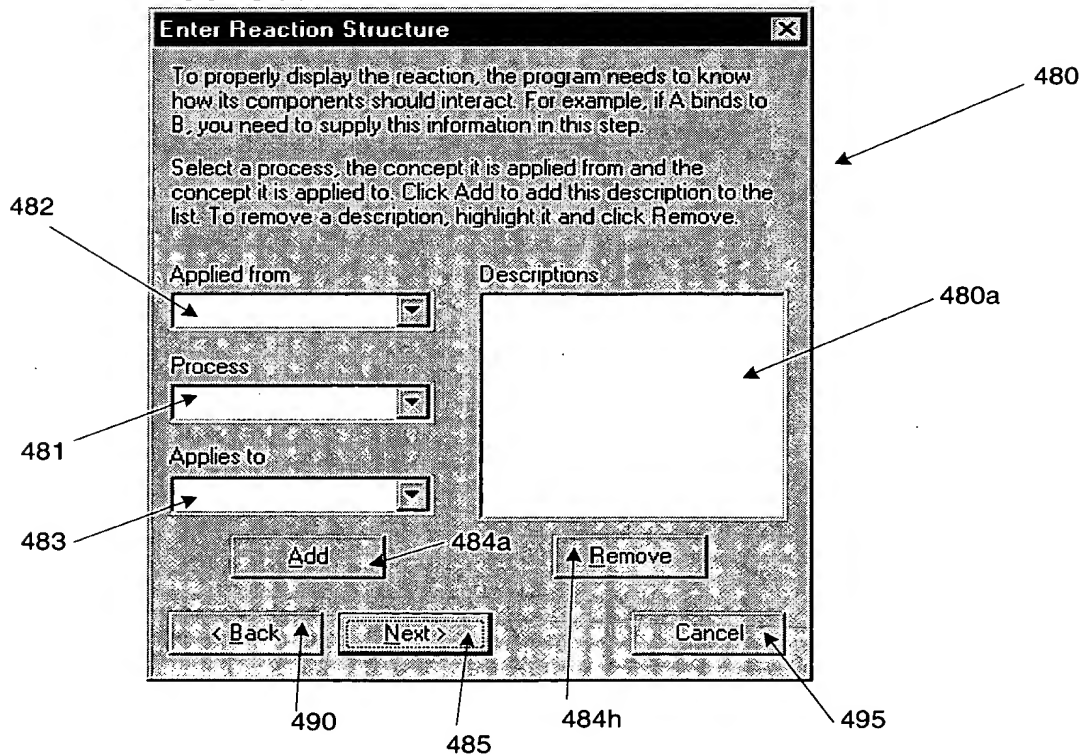


FIGURE 6F

Enter Event Attributes

Events have certain attributes assigned to them that associate information with them. In the space below, enter the values of any relevant attributes for this event.

Event Duration seconds

To provide the best dynamic representation of a reaction, information about the mobility and post-reaction presence of the reactants is needed. Select each reactant in the list below, and check the relevant boxes.

A2aR
adenosine

☒ Reactant will move during the reaction towards other reactants

☒ Reactant is unchanged by the reaction and should be visible post-reaction

< Back Next > Cancel

FIGURE 6G

Enter Event Contexts

Some reactions may be present or absent for certain cell types. Highlight the cell types for which this reaction is present. If you do not select any, it will be present for all cell types.

breast cancer cell
generic cell
generic cell with FADD
HEK-293 cell

Highlight the cell types for which this reaction is absent. If you do not select any, it will be present for all cell types.

breast cancer cell
generic cell
generic cell with FADD
HEK-293 cell

< Back Next > Cancel

FIGURE 6H

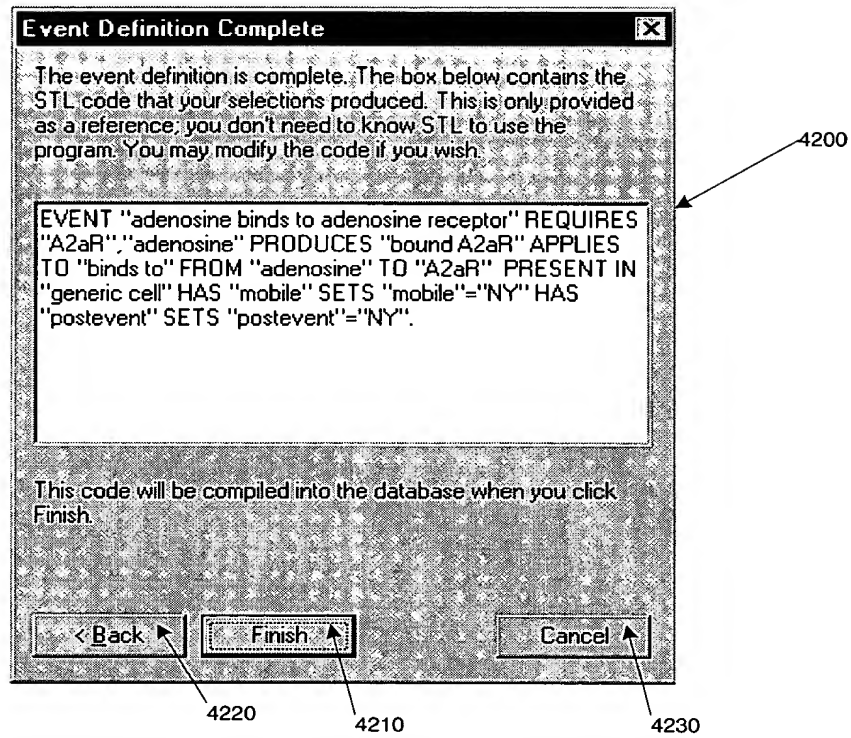


FIGURE 7

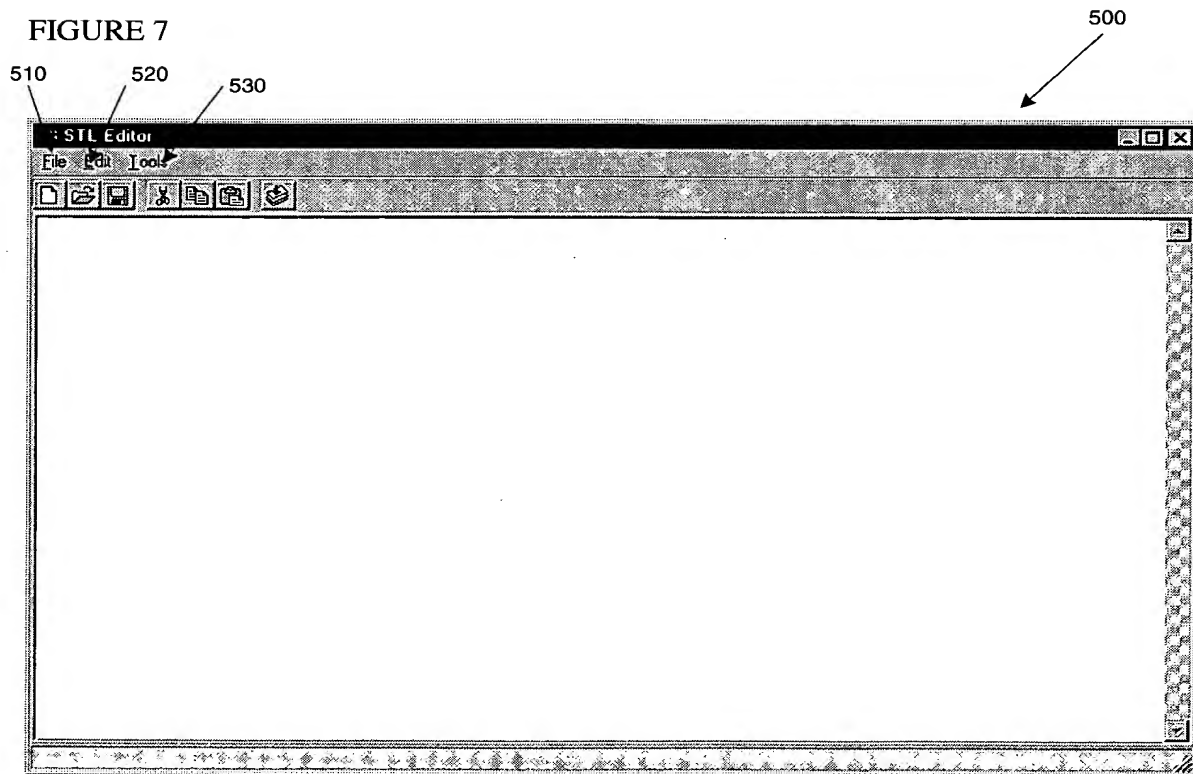


FIGURE 8A

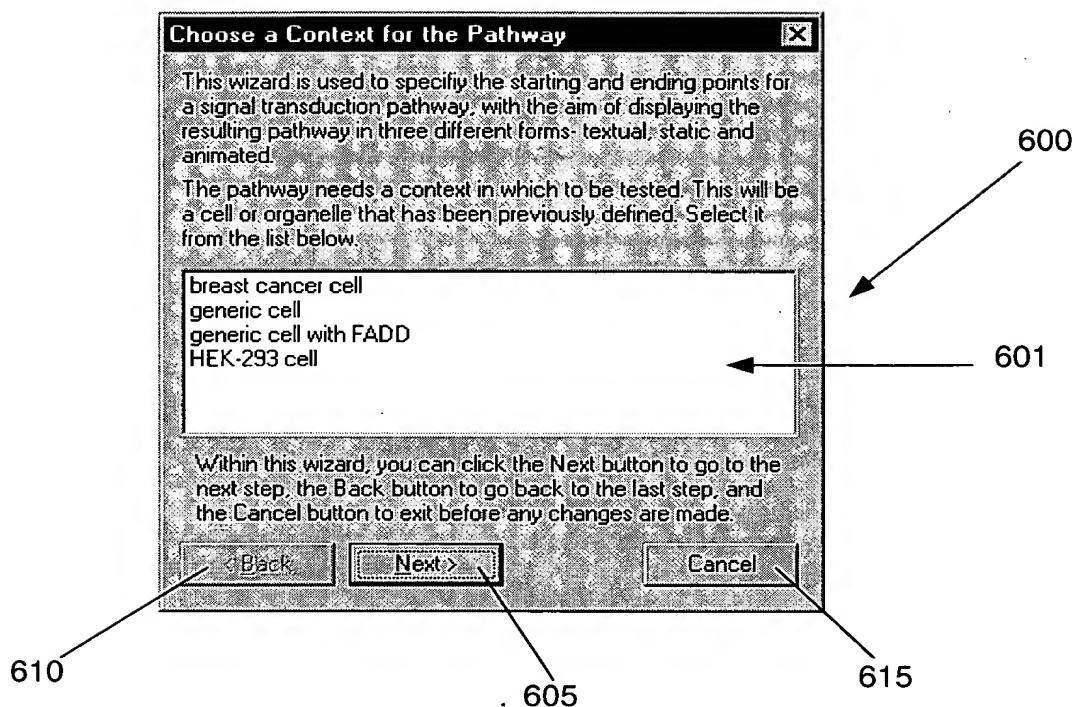


FIGURE 8B

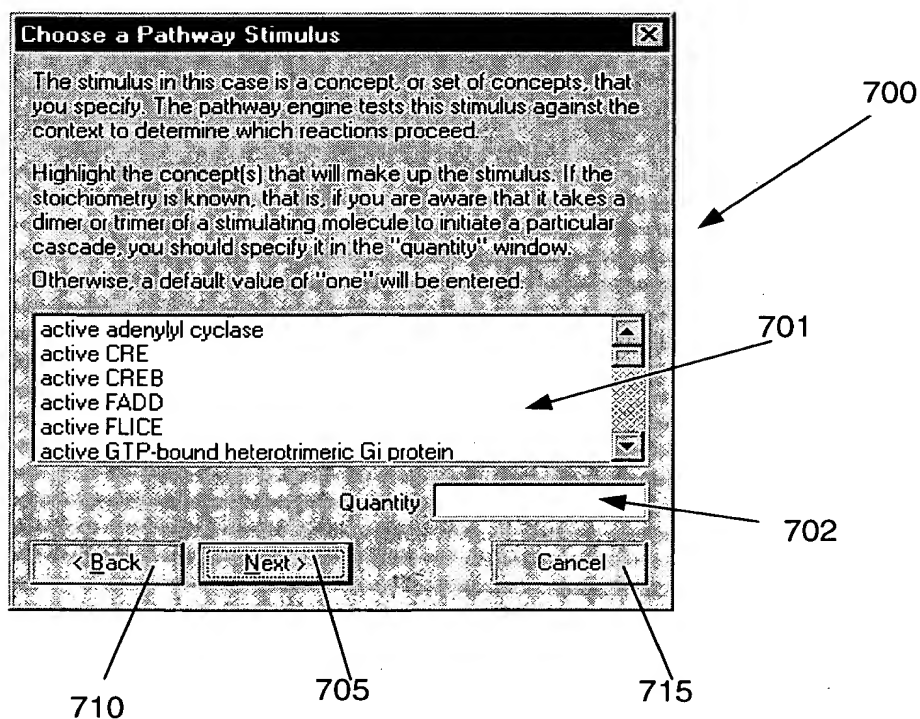


FIGURE 8C

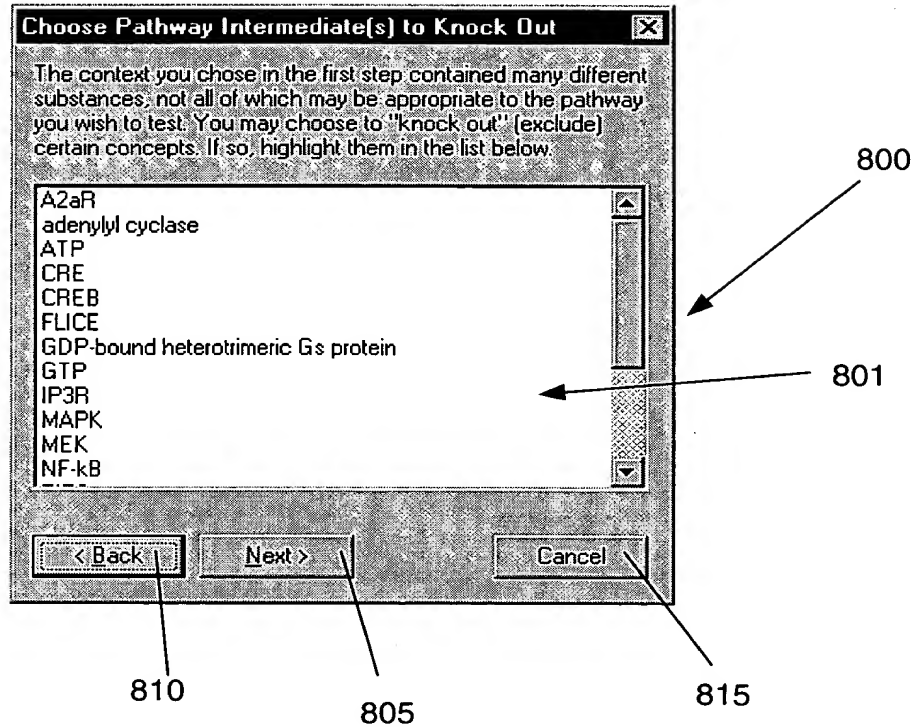


FIGURE 8D

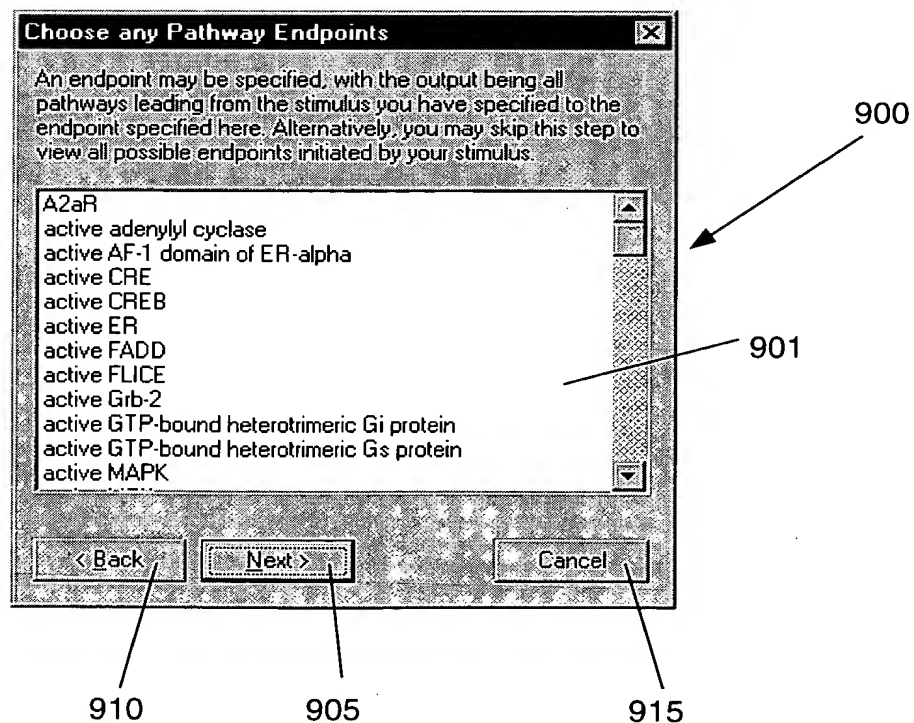


FIGURE 8E

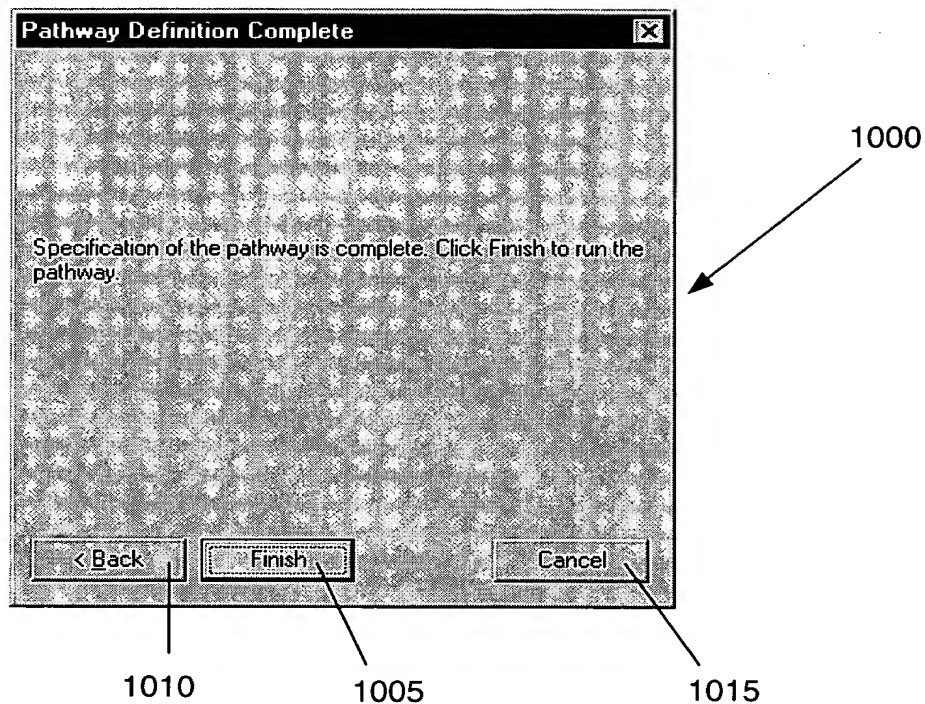


FIGURE 9

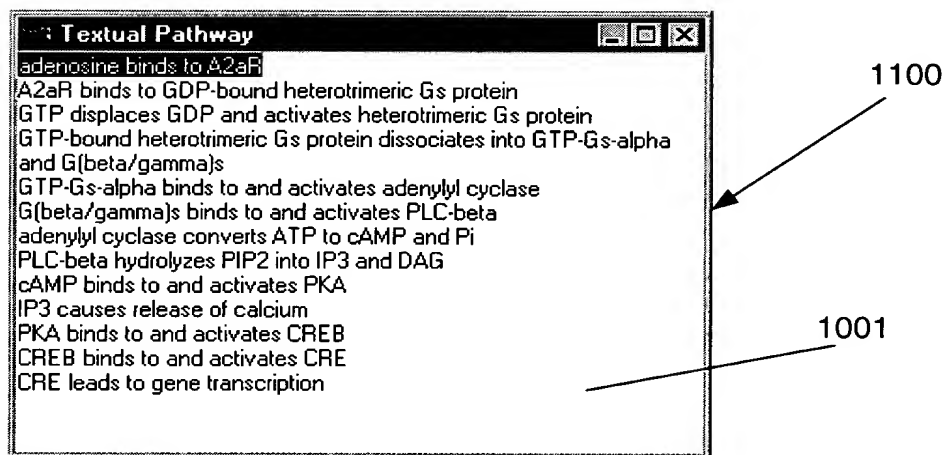


FIGURE 10A

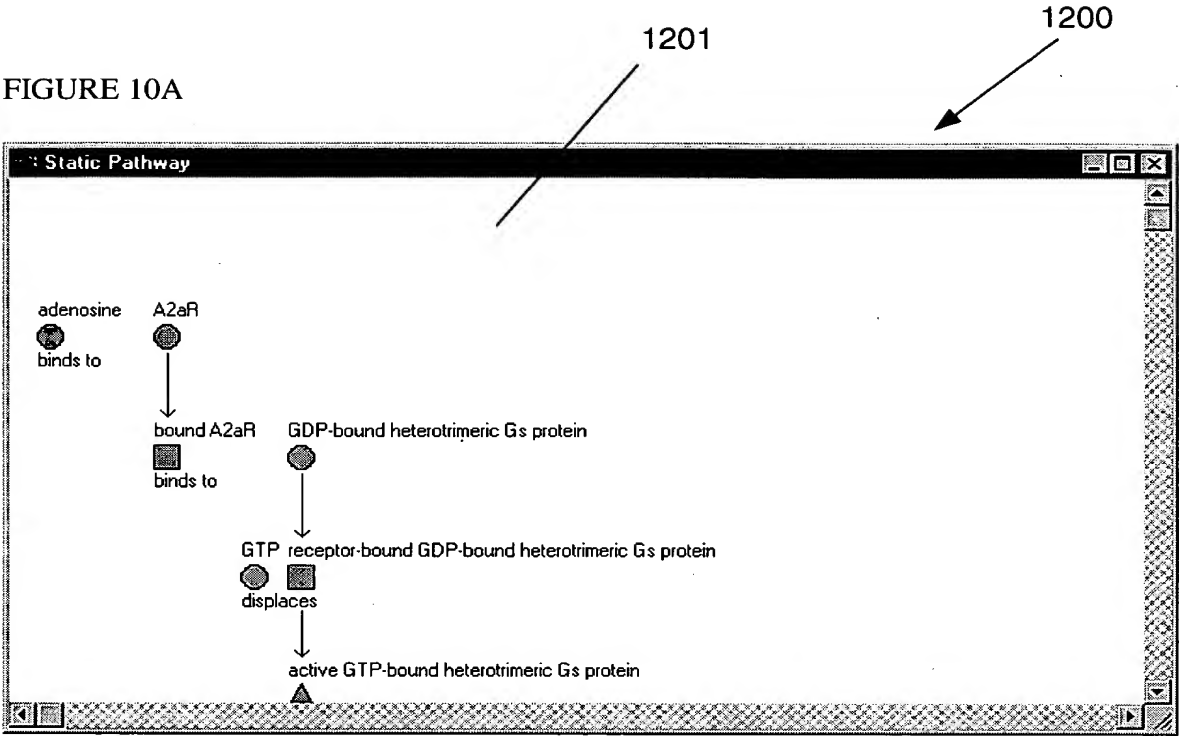
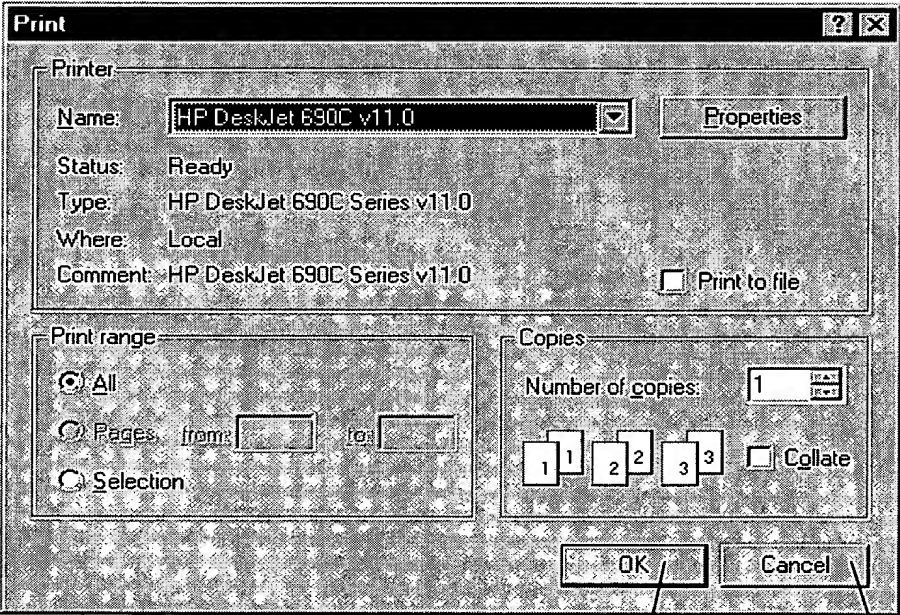


FIGURE 10B



1300

1305

1315

FIGURE 11

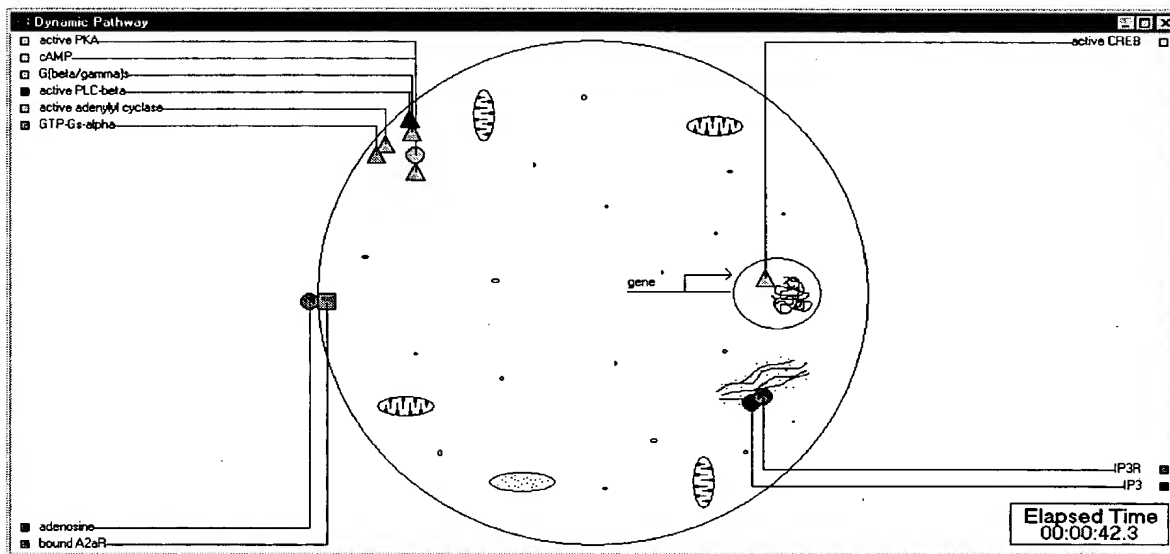
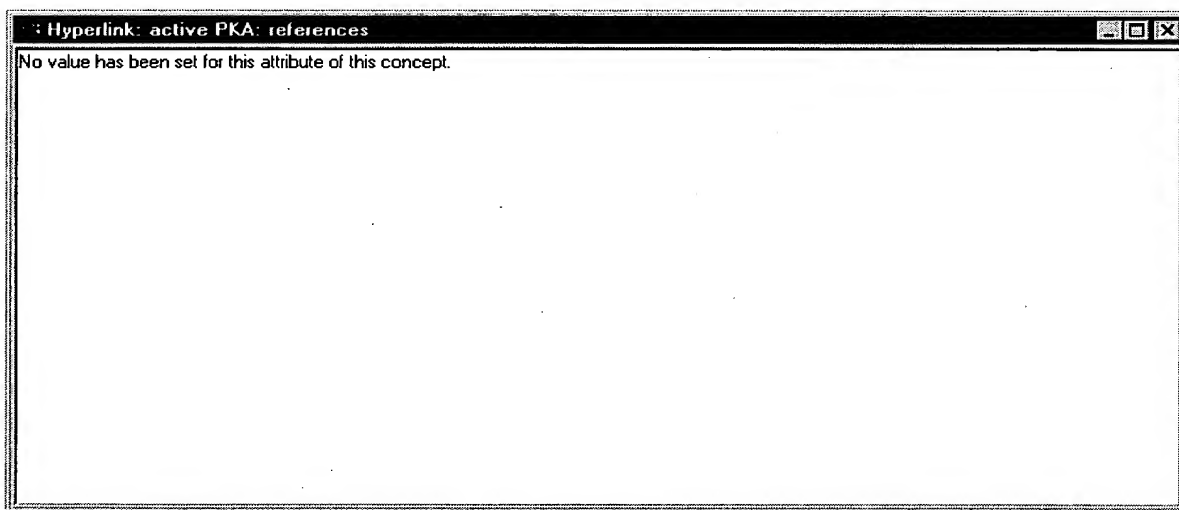


FIGURE 12



5101

Fig. 13

5102

5100

5110

5104

5103

Fig. 14

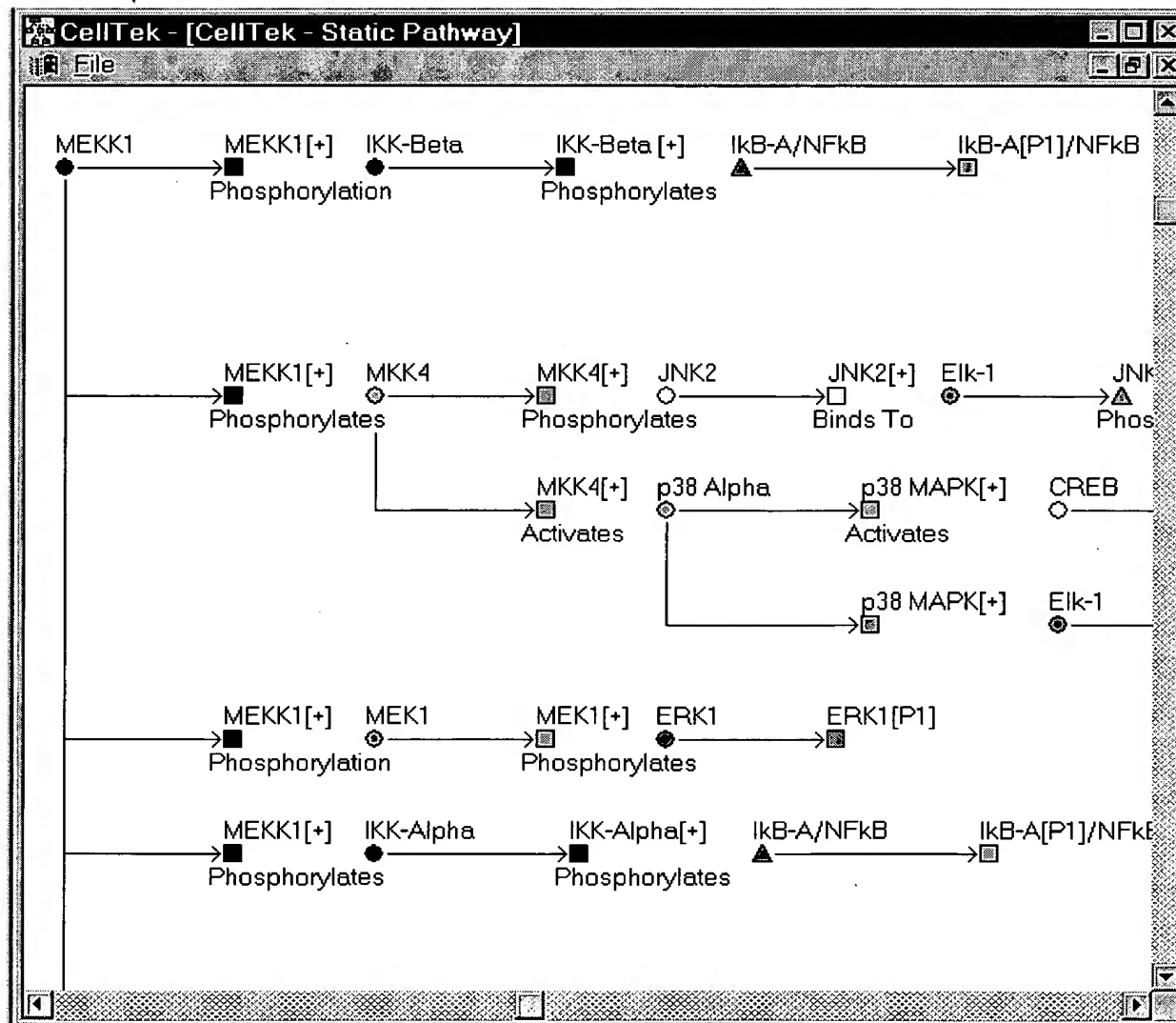


Fig. 15

5120

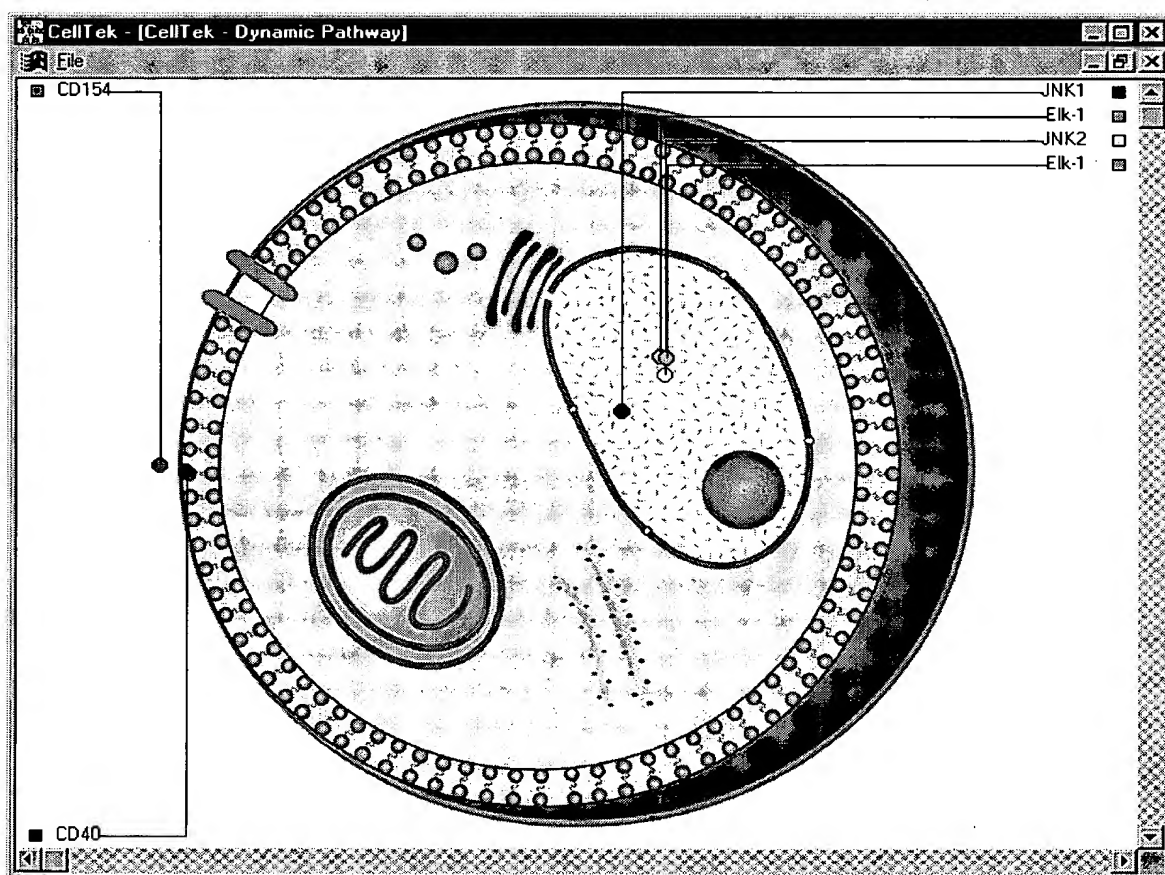
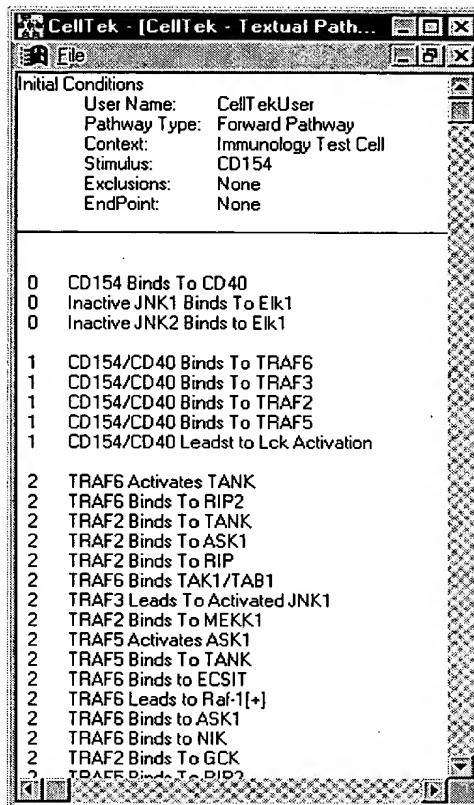
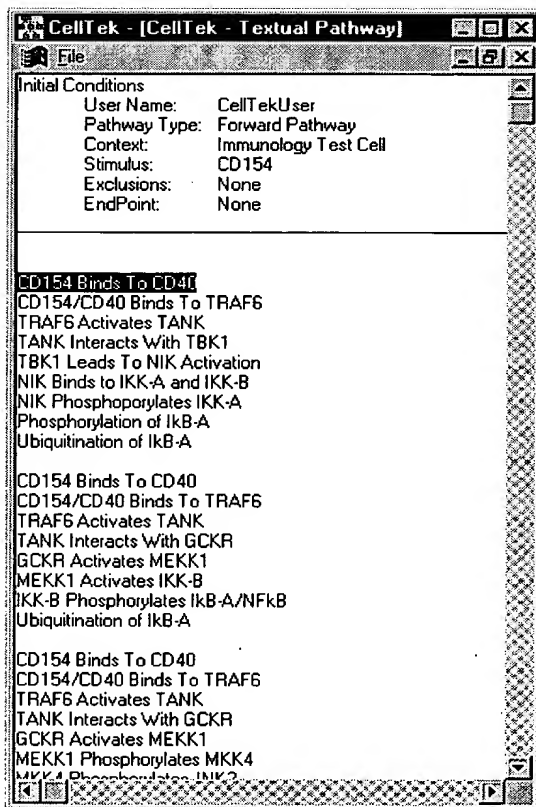


Fig. 16



5140

Fig. 17



5130

Fig. 18

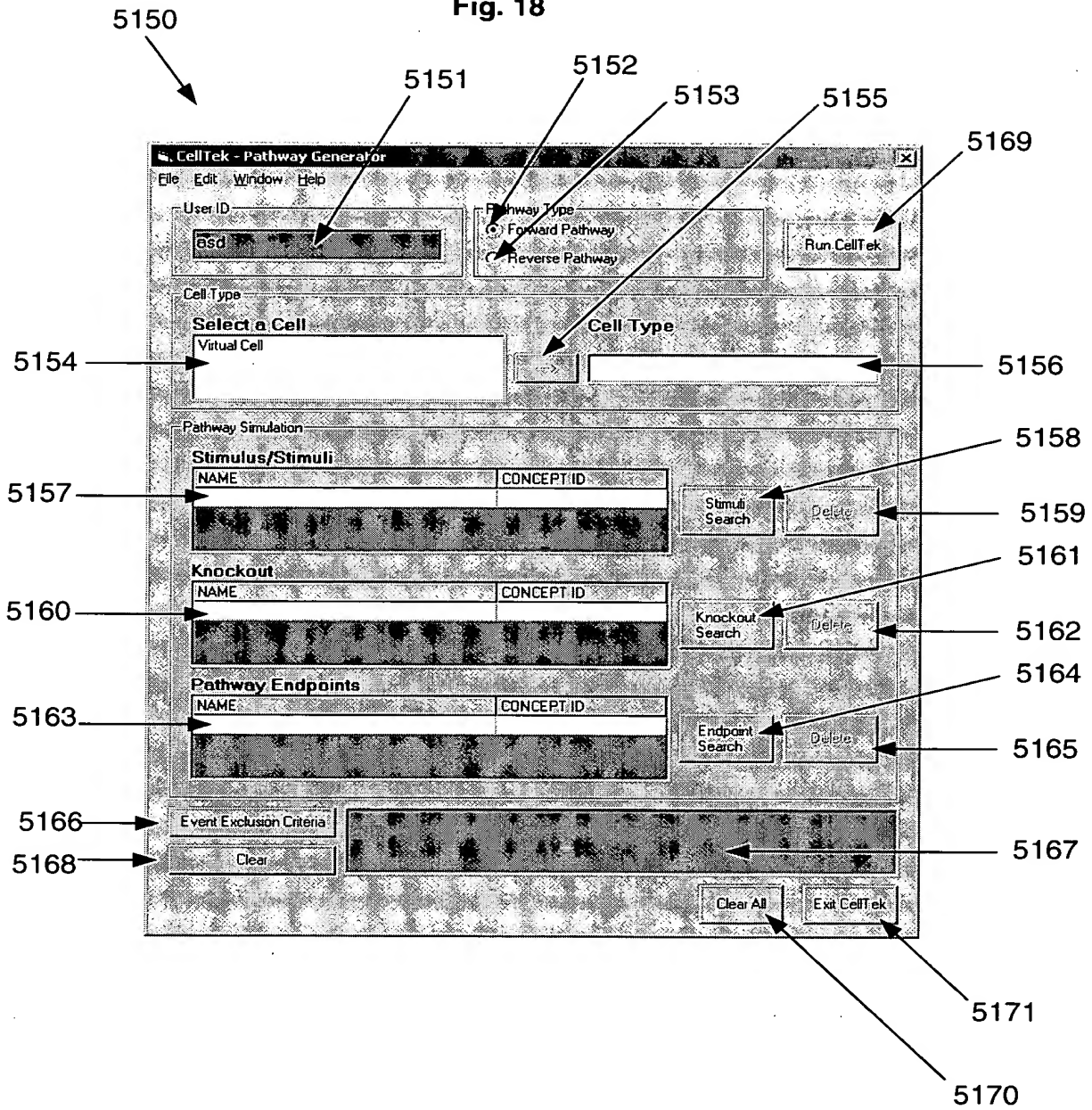


Fig. 19

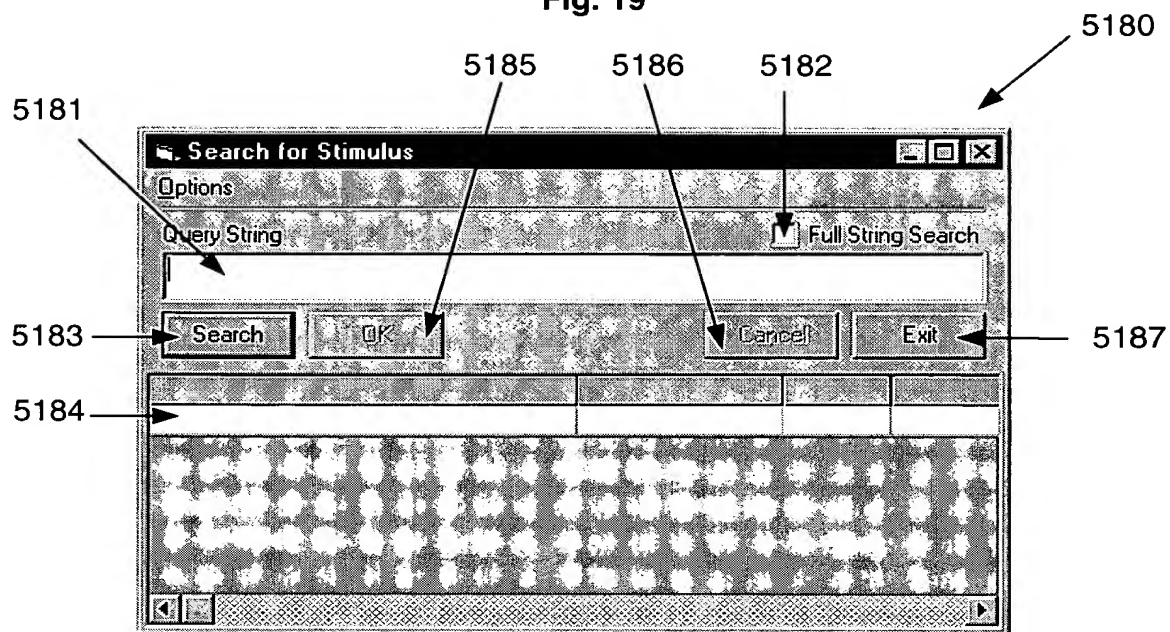


Fig. 20

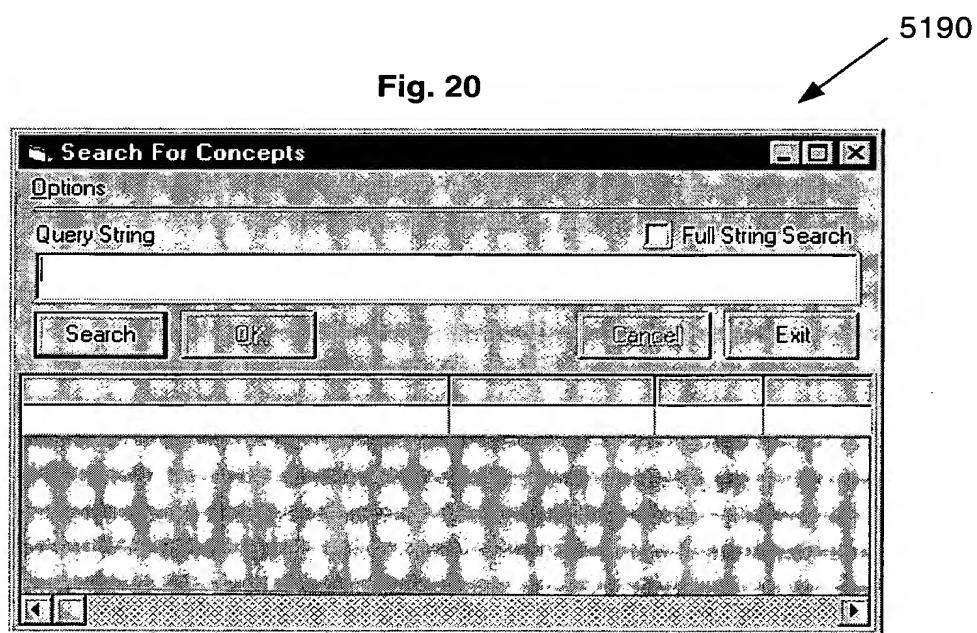


Fig. 21

5200

The dialog box titled "Search for Pathway Endpoints" contains an "Options" section with a "Query String" input field and a "Full String Search" checkbox. Below these are four buttons: "Search", "OK", "Cancel", and "Exit". At the bottom, there is a large, empty rectangular area, likely for displaying search results.

Fig. 22

The dialog box titled "Event Exclusion Criteria" features a "More<<" button at the top left. The main area is organized into four columns: "Fields", "Qualifier", "Values", and "Operator". Each column contains a list of items, with "Fields" and "Qualifier" having dropdown arrows. The "Values" column includes a "Search" button for each entry. The "Operator" column also has a "Search" button. At the top right are "Cancel" and "OK" buttons. Labels with arrows point to specific elements: 5210 points to the "Fields" column, 5211 to the "More<<" button, 5212 to a field in the "Fields" column, 5213 to a field in the "Qualifier" column, 5214 to a field in the "Values" column, 5215 to a "Search" button in the "Values" column, 5216 to a field in the "Operator" column, 5217 to the "OK" button, and 5218 to the "Cancel" button.

Fig. 23

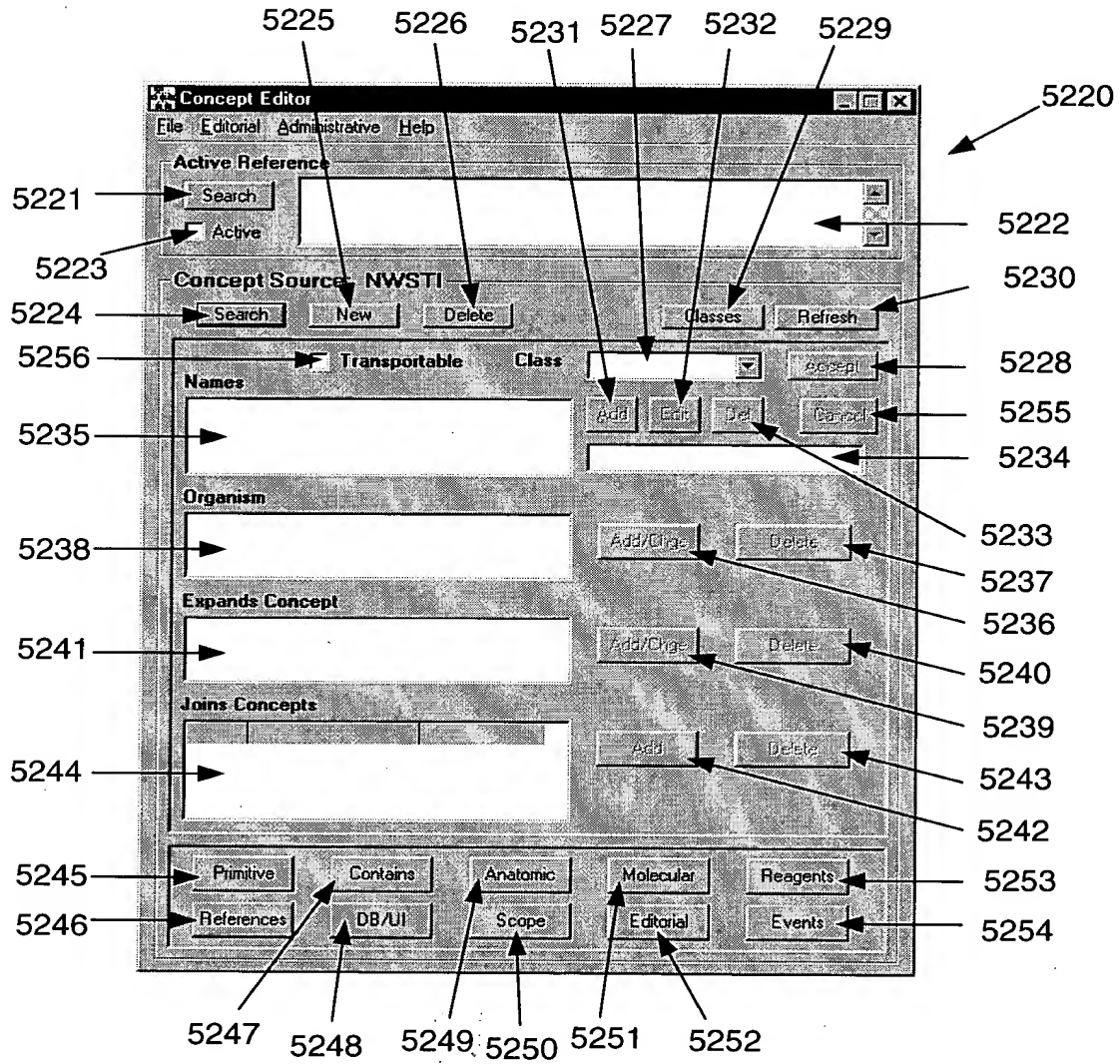


Fig. 24

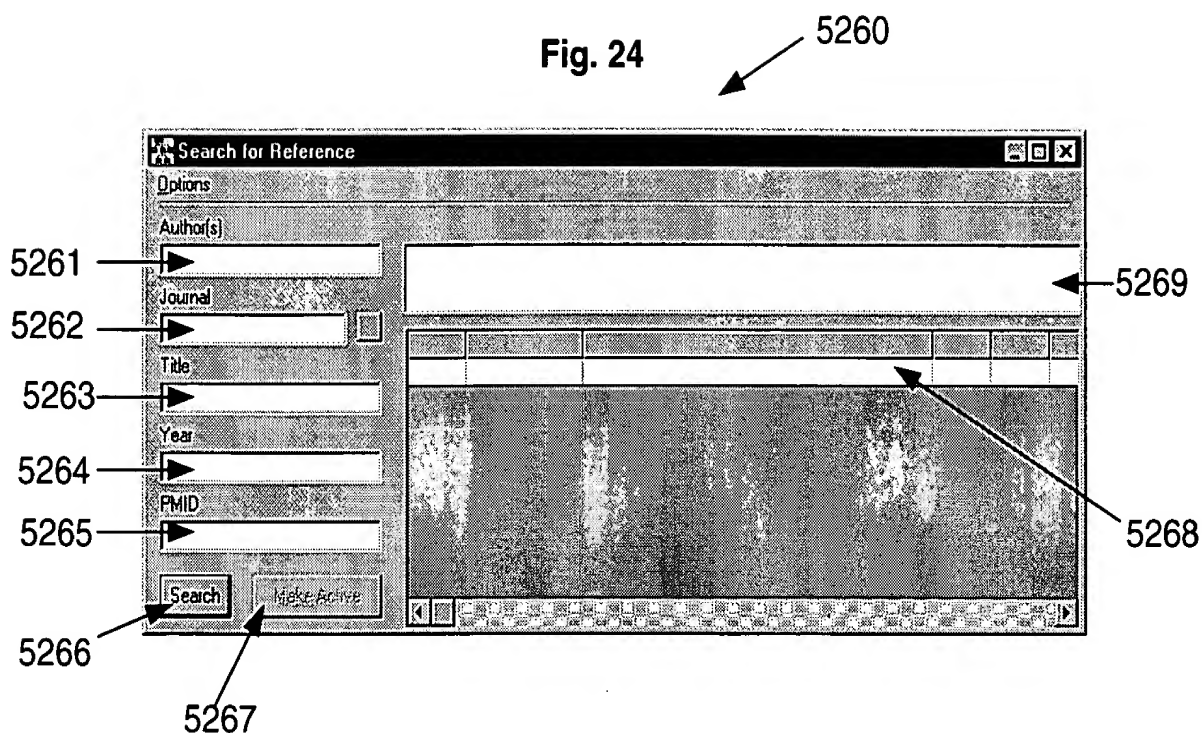


Fig. 25

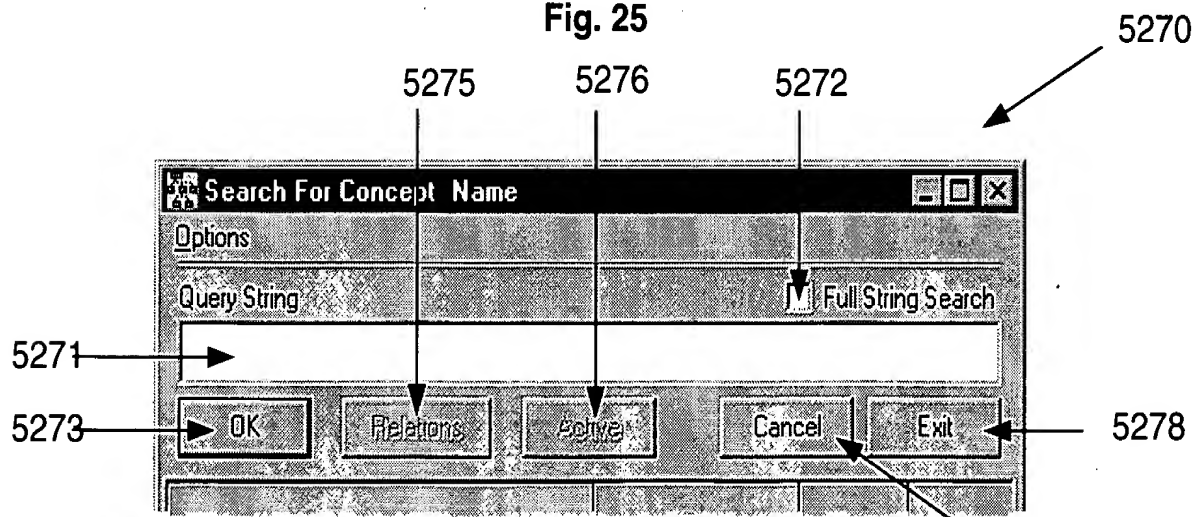


Fig. 26

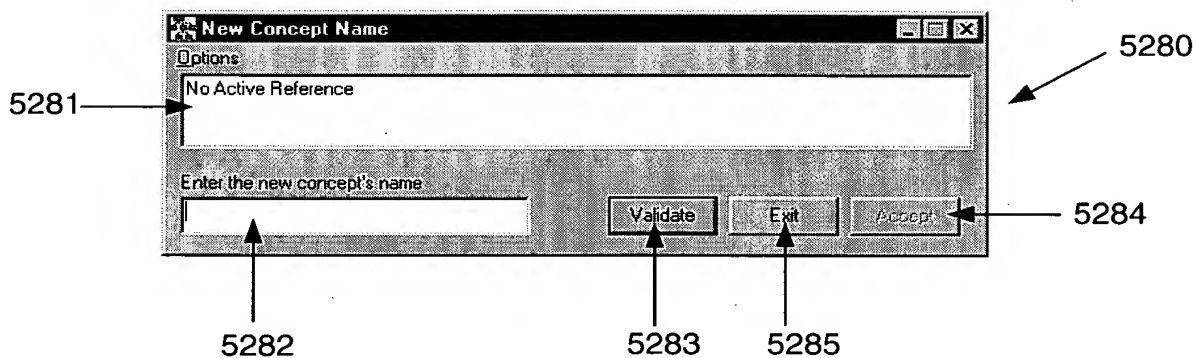


Fig. 27

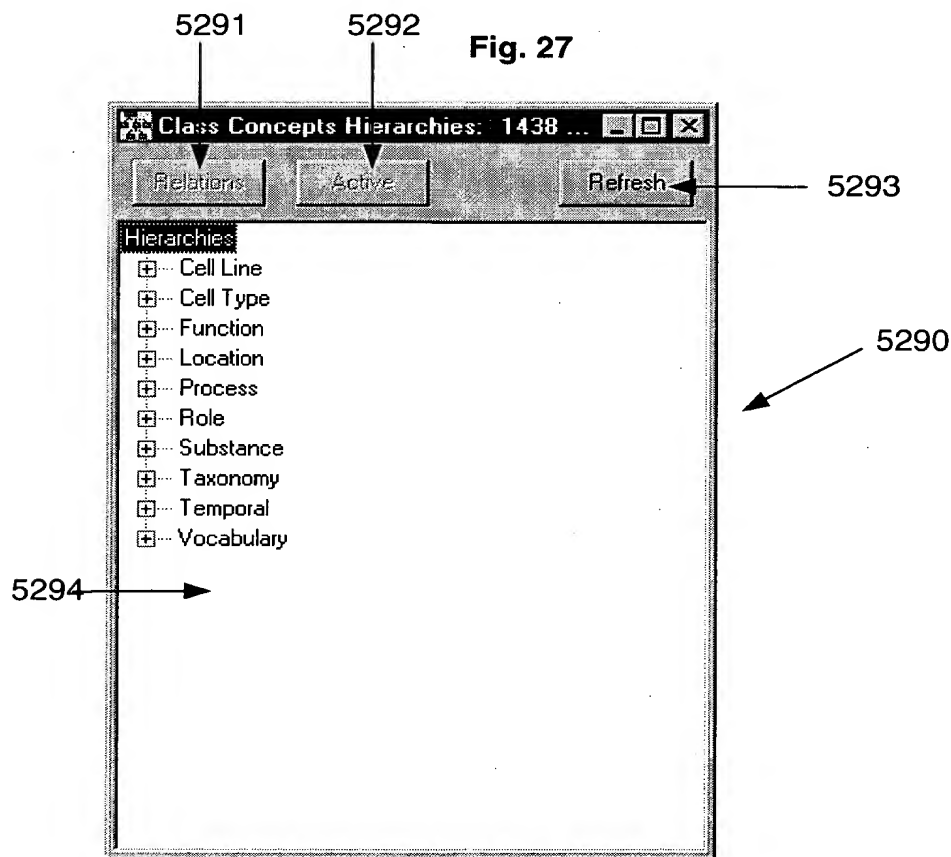


Fig. 28

Primitive Attributes: Concept "TRAF6/T6BP Complex" [X]

ATT ID	Name	Val
5	graphicshape	triangle
6	graphicsize	10
7	graphiccolor	4210688
11	stimulus	1

[Add] [Delete] [Refresh] [Exit]

5300

Fig. 29

Contains - Excludes: Concept "Leukocyte" [X]

Options

[Search] [Refresh] [Exit]

Contains Concepts

--	--

[Add] [Delete] [Delete]

Excludes Concepts

--	--

[Add] [Delete] [Delete]

5310

Fig. 30

Query: Concept "Leukocyte"

Options

Organism

☒ Include ☐ Exclude

Add Delete

Query

Anatomic

☒ Include ☐ Exclude

Add Delete

Query

☐ AND ☒ OR

☐ Dev Stage ☒ Organ ☐ Tissue ☐ Cell Type

Class

☒ Expand

Add Delete

Query

Combinations

☐ Organism - Class ☐ Anatomy - Class

☐ Organism - Anatomy ☒ Org - Anat - Class

Query

Search Refresh

To Contents Exit

5320

Fig. 31

Anatomic Attributes: Concept "Phosphatidylinositol-3-OH-Kinase Family"

No Active Reference

ID	REF_ID	MOL_CELL	STAGE	ORGAN	TISSUE
387	18				

Active ID -
Reference

Developmental Stage

Organ

Tissue

Cell Type

Cell Line

Molecules per Cell

Expression Defined By

5330

Fig. 32

5340

Molecular Attributes: Concept "Phosphatidylinositol-3-OH-Kinase Family"

Member Of Gene/Protein Family

Has A Prototype Homolog

Domains: Active ID - 56

☒ Domains ☐ Motifs ☐ Post-Translational Modifications ☐ Activated By ☐ Inhibited By

ID	DOMAIN_NAME
56	Kinase Domain
57	PIK Domain

References

ID	JOURNAL	TITLE	Year	Vol	Iss
46	Annu Rev Bi	Phosphoinositide kinases.	1998	67	

Fig. 33

5350

Reagents: Concept "Phosphatidylinositol-3-O..."

No Active Reference

REF_ID	NAME
--------	------

Fig. 34

5360

References: Concept "Phosphatidylinositol-3-OH-Kinase Family"

Add Active To Search Delete Cancel

ID	JOURNAL	TITLE	Year	Vol	Issue	Page	PMID	RFLIST
45	Biochim Bio	Structu	1998	1436	1-2	127	9838078	296

Fig. 35

External Databases: Concept "Phosph..."

Add Delete Refresh Exit

5370

Fig. 36

5380

A screenshot of a software window titled "Scope Notes: Concept 'Phosphatidylinositol-3-O...". The window contains a large text area at the top, a table below it, and a row of five buttons at the bottom: "Add", "Edit", "Delete", "Cancel", and "Exit".

COMMENT_ID	COMMENT	ID	COMMENTTYPE_ID	COMMENTREFT
[Empty table body]				

Fig. 37

5390

A screenshot of a software window titled "Editorial Comments: Concept 'Phosphatidylinosit...". The window contains a large text area at the top, a table below it, and a row of five buttons at the bottom: "Add", "Edit", "Delete", "Cancel", and "Exit".

COMMENT_ID	COMMENT	ID	COMMENTTYPE_ID	COMMENTREFT
[Empty table body]				

Fig. 38

Event Editor: Concept "CD154, Protein"

Administrative

Active Reference
No Active Reference

Event

ID	NAME
42	CD154 Binds To CD40
315	Test Event

Buttons: Refresh, Exit, Constants, Experimental, Attributes, Containers, References, DB / UI, Editorial, Scope, New Event, Delete, Search Event.

Names
Test Event Event Desc

Buttons: Add, Delete, Edit, Cancel

Requires

Produces

Controversy Flag ☐ **Search Concept**

Inhibited By

Cellular Location

Transportable Cellular Location

Buttons: Add, Delete

5405

5400

Fig. 39

Search For Event Name

Options

Query String ☐ Full String Search

Buttons: OK, Active, Cancel, Exit

Table:

Buttons: First, Last

Fig. 40

Biochemical Constants: Event "Test Event"

Active Reference
No Active Reference

Vmax

Km

Keq (Equilibrium Constant)

Kd (Dissociation Constant)

k+1 (Forward Rate)

k-1 (Reverse Rate)

☐ Kinetic Display

☐ Completed Constants

5410

5420

Fig. 41

Event Attributes: Event "Test Event"

Event Name
Test Event

Has Attributes

ID	Name	Val

Applies Process

ID	FROM	APPLIES	TO

Tests Attributes

ID	ATT_1	CON_1	COMPARE	ATT_2	CON_2

Modifies Attributes

ID	CONCEPT	ATTRIBUTE	OPERATOR	VALUE

Fig. 42

5430

Experimental Conditions: Event "Test Event"

Active Reference
No Active Reference

Refresh
Exit

Experimental Conditions

EXP_ID	REF_ID	ASSAY_ID	ASSAY_PRI	BUFFER	PERATURE	RATION_ID

New
Delete

Reference

Assay Name

Add/Change
Delete

Sample Preparation Type

Add/Change
Delete

Assay Description: Processing/Procedure

Accept
Delete

Assay Buffer

Accept
Delete

Temperature C

Accept
Delete

Fig. 43

5440

Excluded: Event "Test Event"

Search
Refresh
Exit

Excluded From

Add
Delete
Details